Supporting Information

A Selective Hydrofunctionalization of *N*-Allenyl Derivatives with Heteronucleophiles Catalyzed by Brønsted Acids

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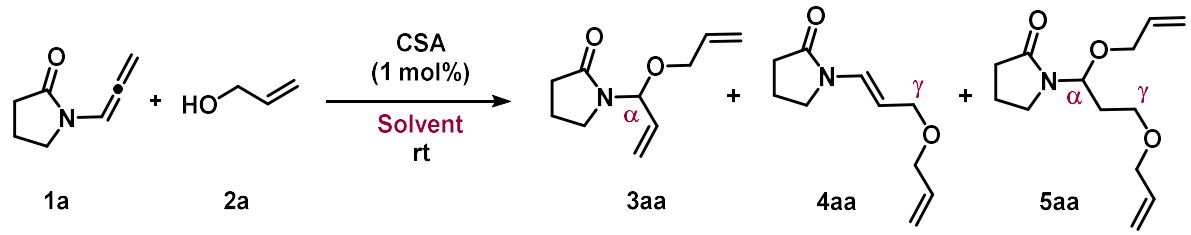
1. Optimization of the Reaction Conditions

1. Solvents Screening

While anisole (PhOMe) and DCM gave good results, other tested solvents were not suitable for this reaction. In particular DMF and DMSO gave average and high conversion of the starting material, respectively (entries 2-3, Table S1), but in both cases no desired product was observed. Better results were obtained with toluene (entry 5, Table S1) but still with lower yield compared to anisole.

Table S1. Further solvents screening.[a]



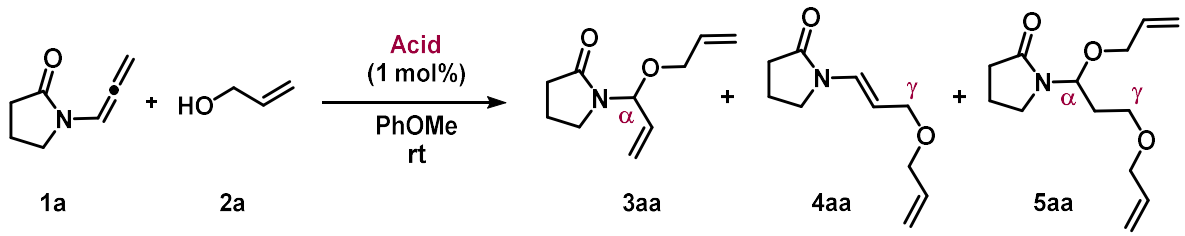
Entry	Solvent	Time [h]	Conversion [%][b]	Products Yield [%][b]		
				3aa	4aa	5aa
1	DCM	3	94	6	72	-
2	DMF	3	46	-	-	-
3	DMSO	3	73	-	-	-
4	PhOMe	2	98	5	70	10
5	PhMe	2	87	25	37	-

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (1.2 eq.), CSA (1 mol%, stock solution 0.025 M in the reaction solvent), solvent (0.2 M), rt. [b] Conversion and products yield determined by ^{1}H-NMR analysis of the crude using methyl acetoacetate as internal standard. eq. = equivalents, DCM = dichloromethane, rt = room temperature, h = hours, CSA = (1*S*)-(+)-10-camphorsulfonic acid, DMF = *N*,*N*-dimethylformamide, DMSO = Dimethyl sulfoxide, PhOMe = Anisole, PhMe = Toluene.

2. Catalytic Acids Screening

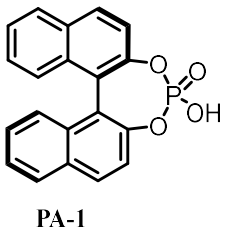
All the other tested acids were not suitable for our reaction, in all cases average to high conversions of the starting material were observed but no product or low yields were obtained.

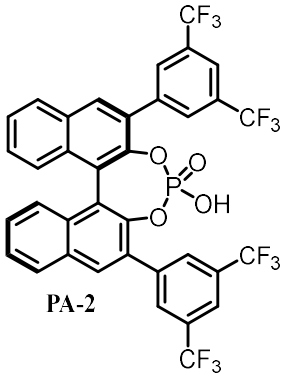
Table S2. Screening of catalytic acids in anisole.[a]



Entry	Acid	Time [h]	Conversion [%][b]	Products Yield [%][b]		
				3aa	4aa	5aa
1	BzOH	2	50	-	-	-
2	AcOH	2	64	-	-	-
3	HCl (37%)	2	68	9	-	-
4	HCl·Et_2O (1M)	2	76	15	-	-
5	PA-1	2	78	25	5	-
6	PA-2	2	95	9	4	-
7	TFA	18	>95	36	14	-

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (1.2 eq.), Acid (1 mol%, stock solution 0.025 M in PhOMe), PhOMe (0.2 M), rt. [b] Conversion and products yield determined by ^{1}H-NMR analysis of the crude using methyl acetoacetate as internal standard. eq. = equivalents, PhOMe = Anisole, BzOH = Benzoic acid, AcOH = Acetic acid.

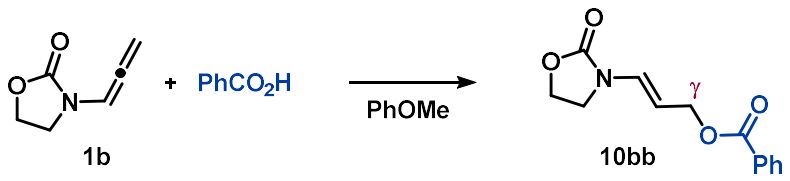




3. Conditions Optimization for the Synthesis of Products **10**

When our standard conditions (1 mol% of CSA at room temperature in anisole) were applied in the presence of benzoic acid as nucleophile, we obtained the desired enamide **10bb** with low yield (entry 1, Table S3). We then tried to increase the nucleophile amount (entries 2 – 3, Table S3), but in all cases only low to average yields and complete conversion of the starting material were obtained. Since allenamide **1b** conversion was complete, we hypothesized a partial substrate degradation, likely promoted by the strong acid employed.[1] Therefore, we decided to avoid the use of strong acids and to directly exploit the nucleophile acidity to activate the allenamide. In the absence of the strong acid and at room temperature a low yield was obtained (entry 4, Table S3), however, the allenamide conversion was not complete. Therefore, we decided to increase the temperature (entries 5 – 7, Table S3) and better results were obtained. The best conditions resulted to be 80 °C in the presence of 3 equivalents of carboxylic acid.

Table S3. Conditions optimization for the carboxylic acids addition.[a]



Entry	CSA [mol%]	$PhCO_2H$ [eq.]	T [°C]	Time [h]	Conversion [%][b]	10bb Yield [%][b]
1	1	1.2	rt	2	>95	34
2	1	2	rt	2	>95	50
3	1	3	rt	2	>95	40
4	-	3	rt	24	60	30
5	-	3	50	5	92	75 (63)
6	-	1.5	50	7	64	45
7	-	3	80	1.5	95	86 (74)

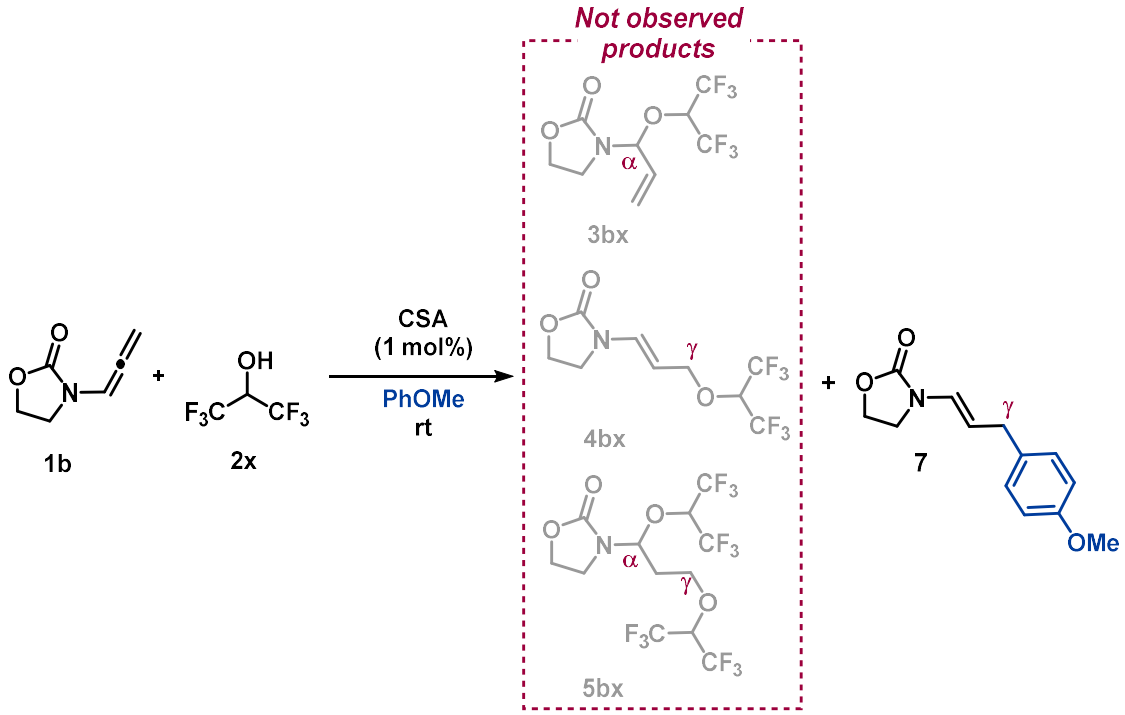
[a] Reaction conditions: **1b** (0.1 mmol), $PhCO_2H$, CSA (1 mol%, stock solution 0.025 M in PhOMe, when indicated), PhOMe (0.2 M). [b] Conversion and products yield determined by ^{1}H-NMR analysis of the crude using methyl acetoacetate as internal standard. Yields after purification in parentheses.

2. Role of HFIP

1. HFIP used as nucleophile, synthesis of product 7

During the investigation of the alcohols scope, we observed that HFIP (1,1,1,3,3,3-hexafluoro-2-propanol) was unable to add to allenamide **1b**. In this case, we isolated compound **7** in a significant yield (entry 1, Table S4), deriving from a Friedel-Crafts addition of the solvent anisole. In order to gain much understanding in the role of HFIP under our conditions, we carried out the reaction in the absence of nucleophile and with an increasing amount of acid catalyst (entries 2 – 3, Table S4). In both cases only a small amount of product **7** was obtained, suggesting a remarkable role of HFIP in the formation of the C–C bond. We attributed this result to the ionizing ability of HFIP which strongly affects the processes generating positively charged intermediates, such as electrophilic aromatic substitutions.[2] Furthermore, HFIP is characterized by a certain acidity (pKa ~ 17.9 in DMSO,[3] pKa ~ 9.3 in water[4]).

Table S4. Evidence on the role of HFIP in the synthesis of product **7**.[a]



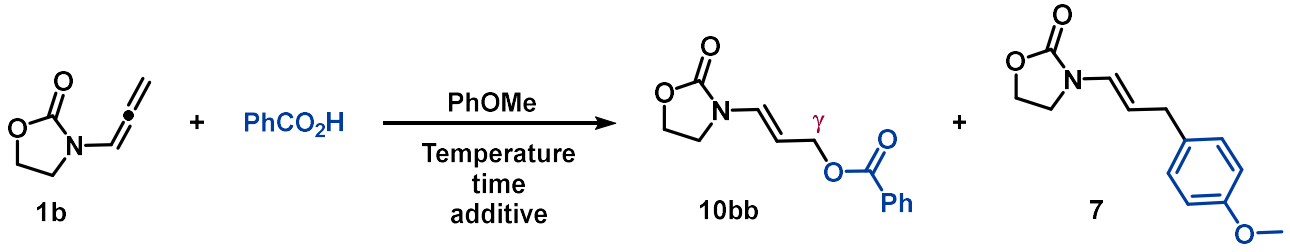
Entry	2x [eq.]	CSA [mol%]	Time [h]	Conversion [%][b]	Products Yield [%][b] 3bx	4bx	5bx	7
1	1.2	1	2	97	-	-	-	56 (52)
2	-	1	2	47	-	-	-	5
3	-	10	2	>95	-	-	-	15

[a] Reaction conditions: **1b** (0.1 mmol), **2x**, CSA (the right amount of a stock solution 0.025 M in PhOMe was added), PhOMe (0.2 M), rt. [b] Conversion and products yield determined by ^{1}H-NMR analysis of the crude using methyl acetoacetate as internal standard. Yields after purification in parentheses.

2. HFIP used as additive with other nucleophiles

In order to gain much understanding in the role of HFIP under our conditions, we used it as additive in presence of other nucleophiles. In particular, we chose two less reactive substrates (benzoic acid and 2-oxazolidinone) that necessitate elevated temperatures for achieving the desired product. We evaluated whether the introduction of HFIP encourages nucleophile addition at lower temperatures or in a shorter time, or if it solely enhances the formation of product **7**.

Table S5. Role of HFIP in the reaction of allenamide **1b** with benzoic acid.[a]



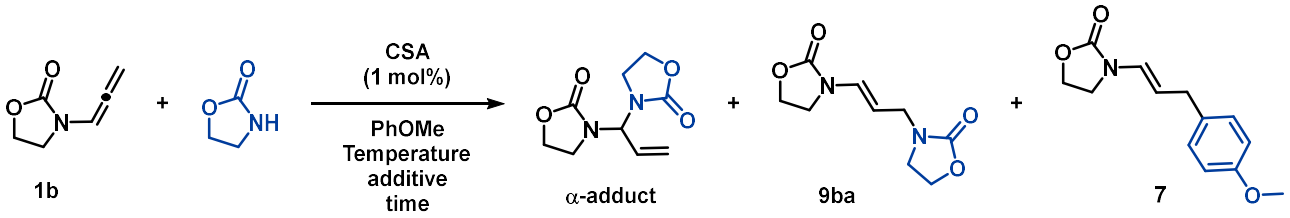
Entry	Time [h]	T [°C]	HFIP [eq.]	Conversion [%][b]	Products Yield [%][b]	
					10bb	7
1	24	rt	-	63	30	-
2	5	50	-	91	78	-
3	1.5	80	-	95	87	-
4	2	rt	1	24	7	-
5	1	80	1	90	68	-
6	2	80	1	>95	79	-

[a] Reaction conditions: **1b** (0.1 mmol), **$PhCO_2H$** (3 eq.), PhOMe (0.2 M), temperature, time. [b] Conversion and products yield determined by ^{1}H-NMR analysis of the crude using methyl acetoacetate as internal standard.

When the reaction between allenamide **1b** and benzoic acid is carried out in presence of 1 eq. of HFIP and at room temperature, only a low yield of the desired product is obtained with no evidence of product **7**. This means that to exploit the acidity of weak acids, it is necessary to increase the temperature also in presence of HFIP (Table S5, entry 4 vs entries 5 and 6). Furthermore, in the absence of the strong acid, HFIP is not able to promote the formation of product **7**. This experimental evidence suggests that the Friedel-Crafts addition of anisole requires both CSA-catalysis and HFIP, according to the already reported cooperation between many Lewis or Brønsted acids and HFIP hydrogen-bond clusters.[5]

On the other hand, when allenamide **1b** reacts with 2-oxazolidinone in the presence of 1 eq. of HFIP at room temperature, an acceleration in the formation of product **7** is noted (Table S6, entry 4). Despite the higher γ/α ratio in entry 4 compared to entry 2, the yield of the desired product is lower due to the generation of **7**. In general, the impact of HFIP under these reaction conditions is to enhance the formation of the Friedel-Crafts adduct, rather than to increase the reaction rate of the formation of product **9ba**. Concerning the oxazolidinone addition, it is important to highlight that the nucleophilic addition catalyzed by CSA is fast, whereas the conversion of α-adduct to γ-adduct is slow and it requires higher temperature.

Table S6. Role of HFIP in the reaction of allene **1b** with 2-oxazolidinone.[a]



Entry	Time [h]	T [°C]	HFIP [eq.]	Conversion [%][b]	Products Yield [%][b]		
					α-adduct	9ba	7
1	2	rt	-	>95	37	53	-
2	5	rt	-	>95	33	49	2
3	3	80	-	>95	6	70	5
4	2	rt	1	95	9	30	24
5	1	80	1	>95	-	30	20
6	2	80	1	>95	-	20	13

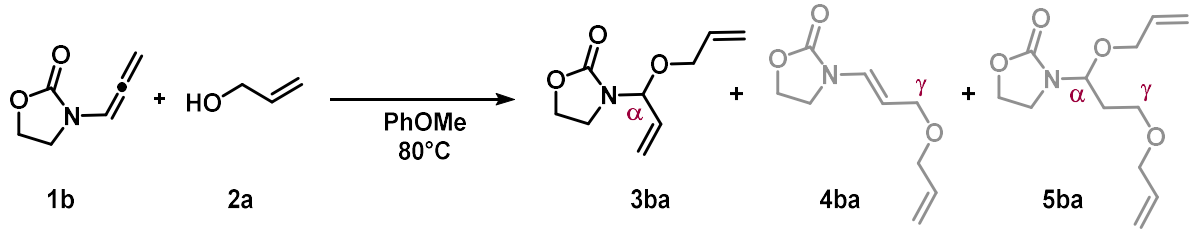
[a] Reaction conditions: **1b** (0.1 mmol), 2-oxazolidinone (1.2 eq.), CSA (1 mol%), PhOMe (0.2 M), temperature, time. [b] Conversion and products yield determined by ^{1}H-NMR analysis of the crude using methyl acetoacetate as internal standard.

3. Mechanistic Studies

1. Reaction without the acid catalyst

In order to demonstrate the role played by the catalytic CSA in promoting the alcohol addition to allenamide, we performed the reaction between allene **1b** and allyl alcohol **2a** in anisole at 80 °C without the acid catalyst. After 6 hours we observed a not full conversion of the starting material **1b**, a small amount of the α-adduct **3ba** and no traces of the desired product **4ba**. It demonstrates the necessity of the acid catalyst to achieve an acceptable yield of the desired enamide **4**.

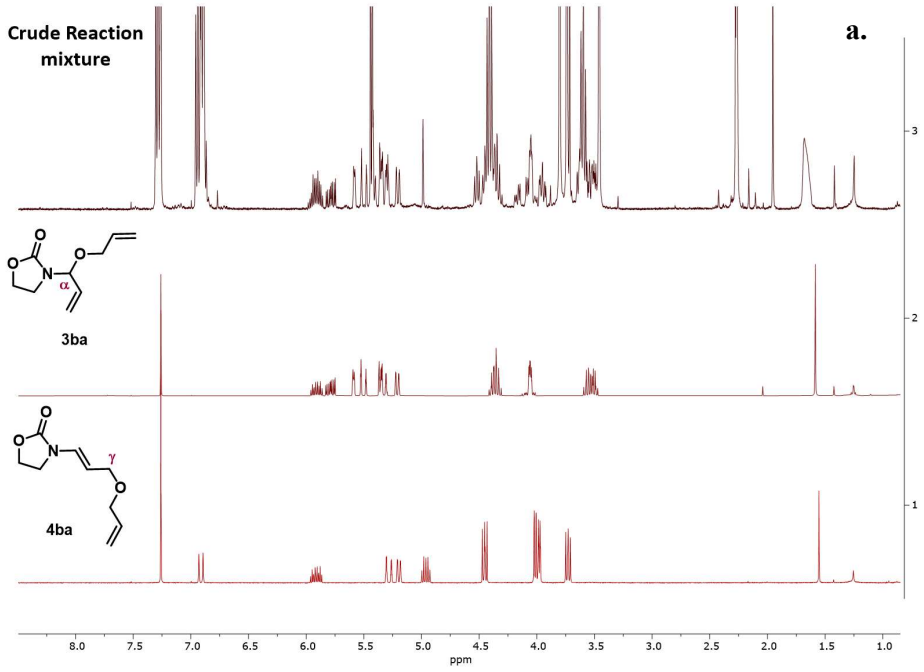
Table S7. Reaction performed in the absence of the acid catalyst.[a]

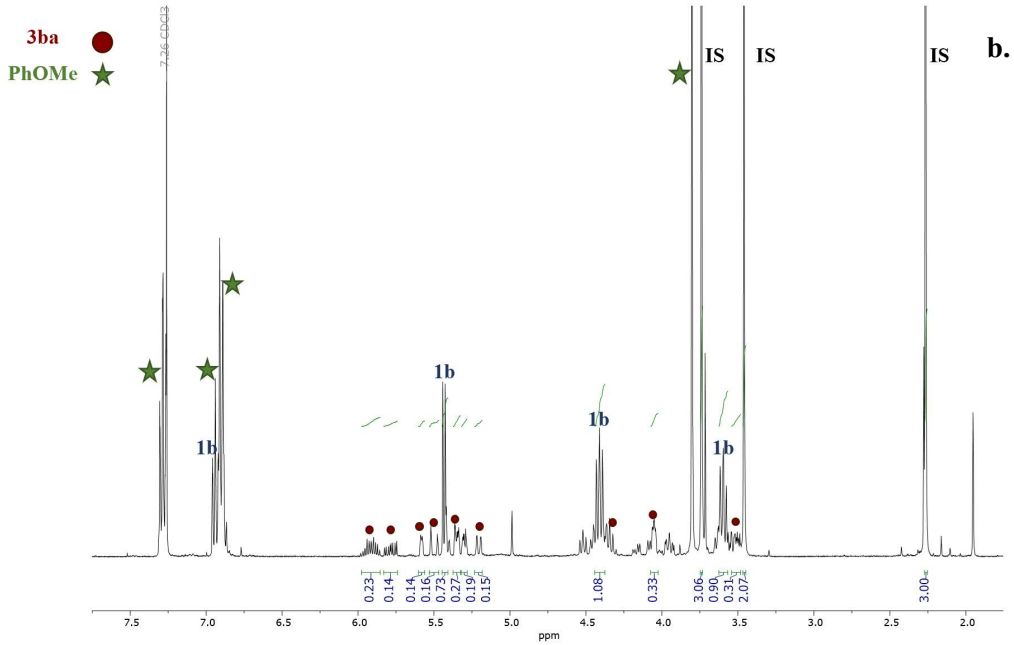


Entry	2a [eq.]	Time [h]	Conversion [%][b]	Products Yield [%][b]		
				3ba	4ba	5ba
1	1.2	5	64	15	-	-

[a] Reaction conditions: **1b** (0.1 mmol), **2a** (1.2 eq.), PhOMe (0.2 M), 80 °C. [b] Conversion and product yield determined by ^{1}H-NMR analysis of the crude using methyl acetoacetate as internal standard.

Figure S1. a. Superimposition of the crude reaction mixture (top) with the purified product **3ba** (centre) and the purified product **4ba** (bottom). **b.** Crude reaction mixture.





2. HRMS analysis of the reaction mixture

In order to gain much understanding on the reaction mechanism, we set up the reaction between allenamide **1b** and allyl alcohol **2a** in anisole under standard conditions (1 mol% of CSA at rt), and we analysed the reaction mixture with high resolution mass spectrometry (HRMS) after 45 minutes.

The HRMS spectra showed the presence of: intermediate **I2** (Figure S2), substrate **1b** (Figure S3), CSA (Figure S4) and the isomeric products **3ba** and **4ba** (Figure S5).

Figure S2. Extraction of the exact mass of intermediate **I2** from the HRMS analysis.

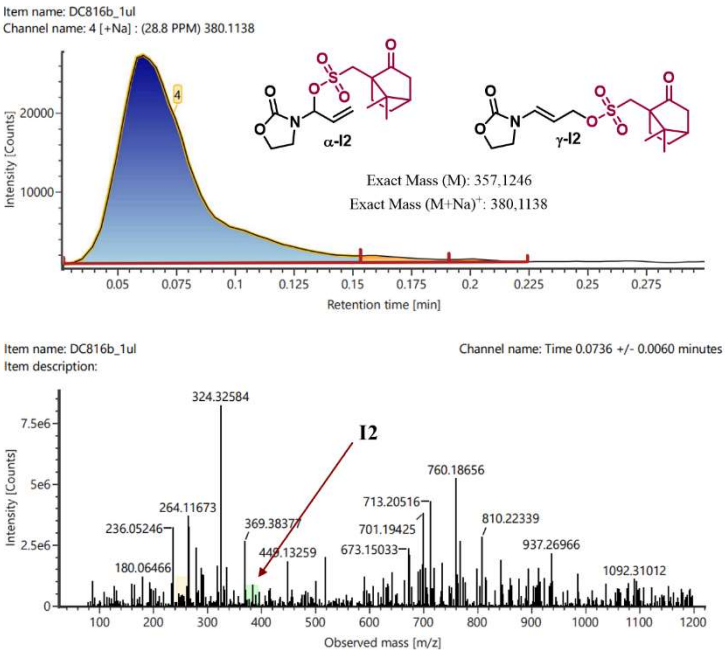


Figure S3. Extraction of the exact mass of **1b** from the HRMS analysis.

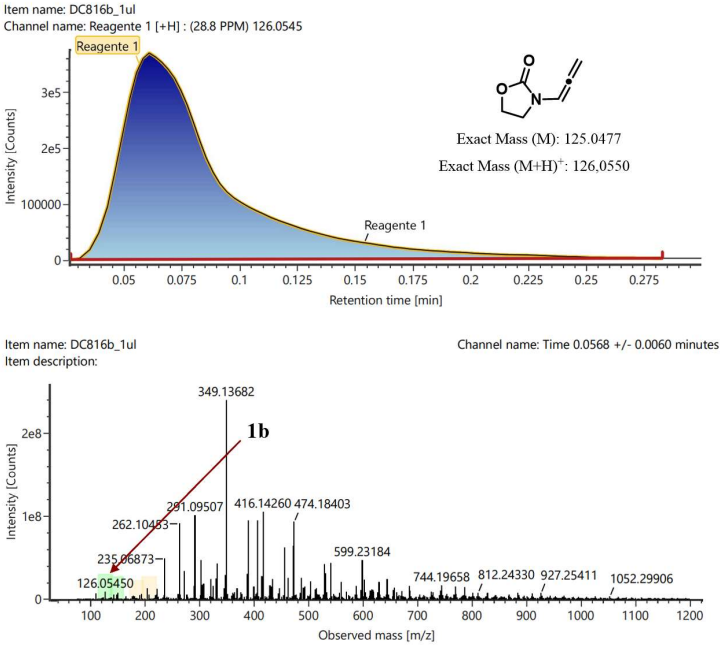


Figure S4. Extraction of the exact mass of **CSA** from the HRMS analysis.

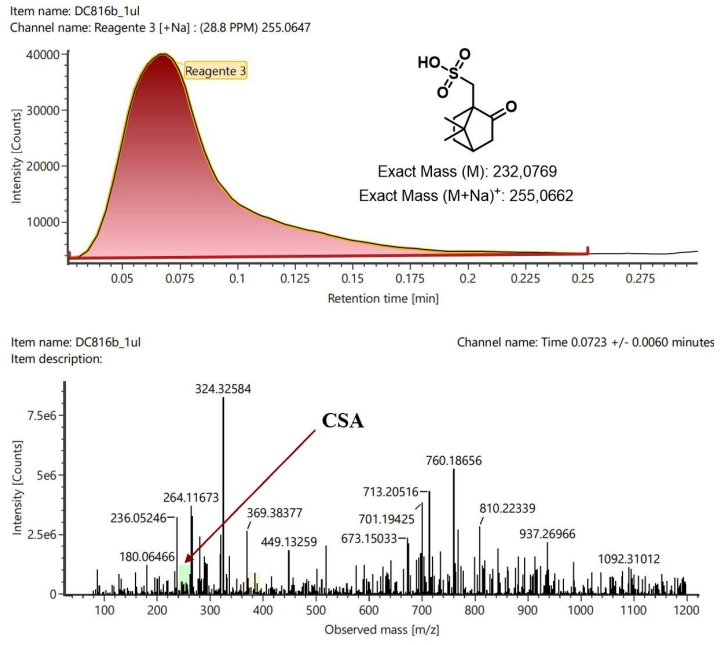
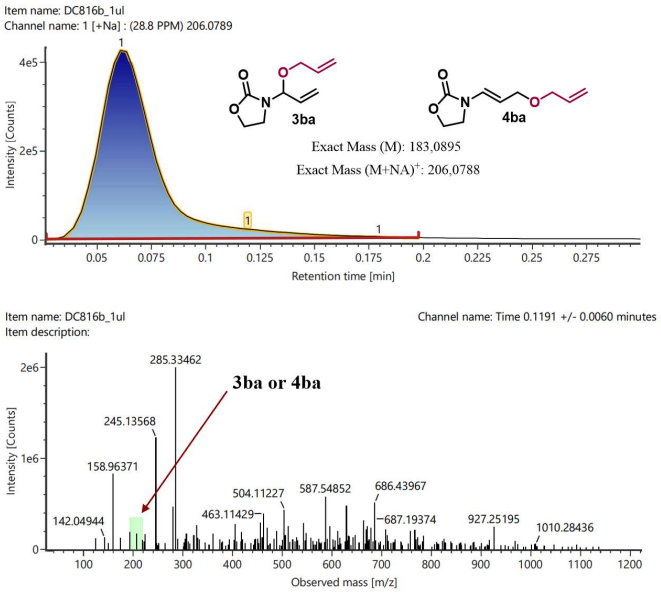


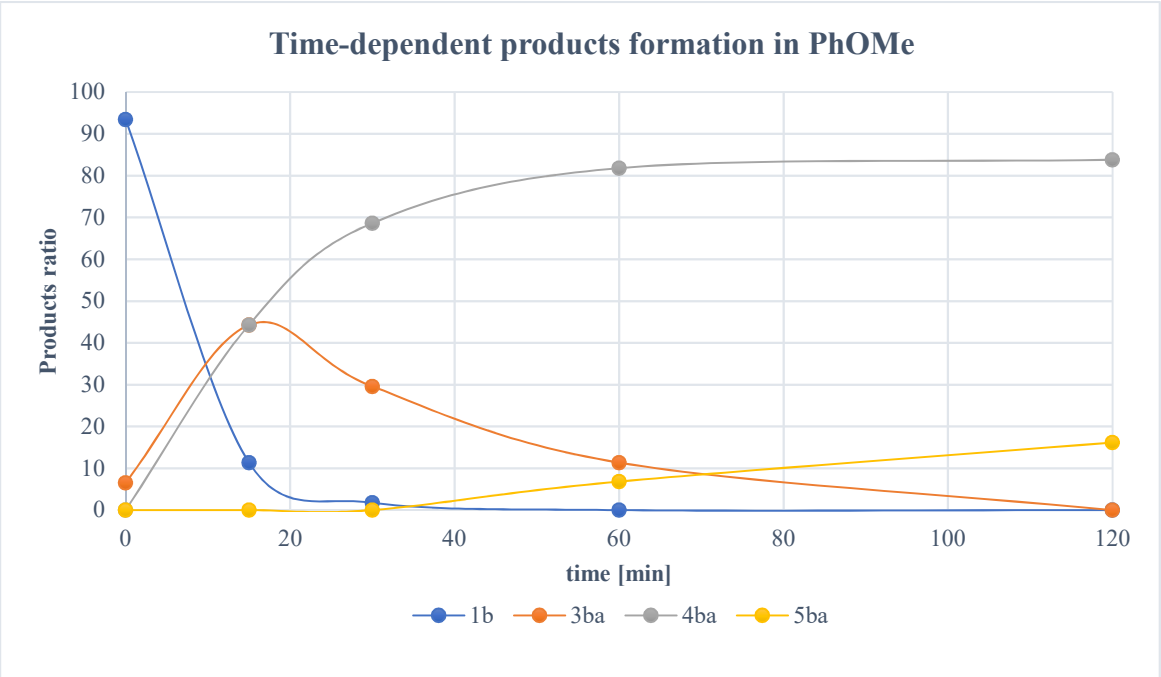
Figure S5. Extraction of the exact mass of products **3ba** and/or **4ba** from the HRMS analysis.



3. Products distribution over time in DCM and PhOMe

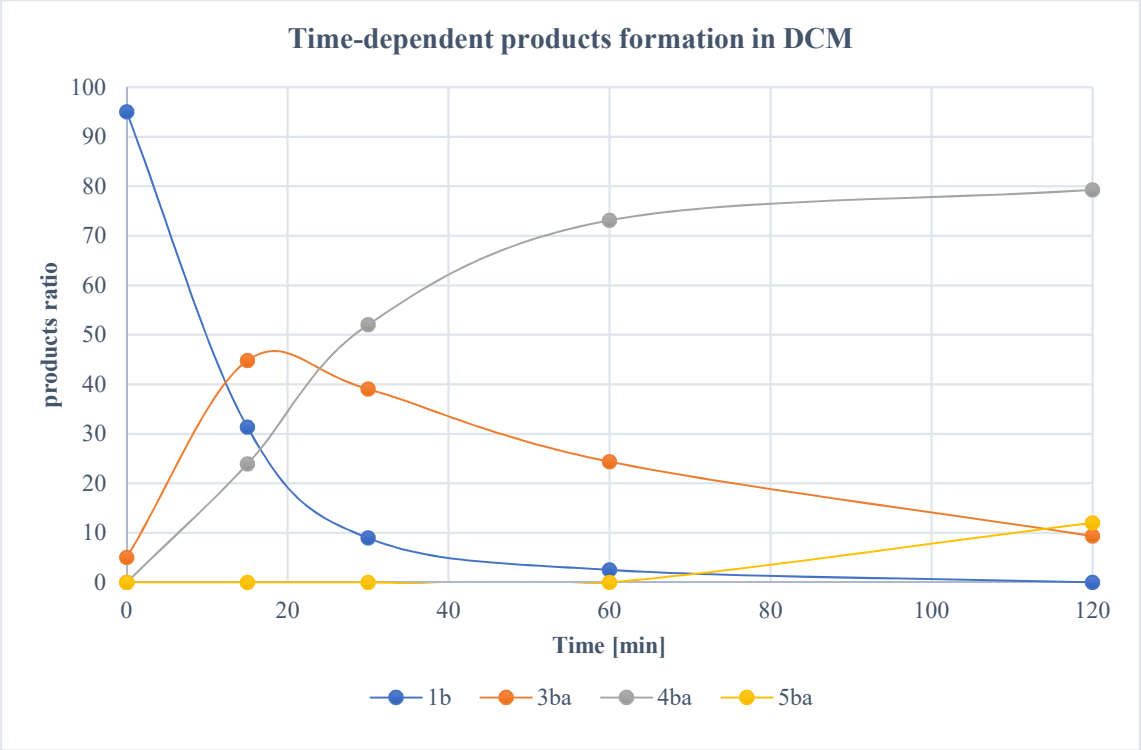
In order to gain much understanding on the reaction mechanism, we studied the products distribution over time in both DCM and PhOMe. In particular, we set up the reaction between allenamide **1b** and allyl alcohol **2a** in the standard conditions and we collected a sample immediately after the addition of the acid, and then others after 15, 30, 60 and 120 minutes. Each sample was quenched as described in the general procedure, then it was analysed by means of ^{1}H-NMR to determine the ratio between allenamide **1b** and products **3**, **4** and **5**. This study demonstrates that the starting material is very quickly consumed leading to the formation of both products **3** and **4**. In particular, the obtained results confirm the kinetically favored formation of **3** and the transformation of **3** into **4**, the amount of which increases over time even after the allenamide disappearance. Moreover, the reaction in anisole exhibits a higher rate compared to that in DCM, as evident from the comparison between the two graphs (Table S8 vs Table S9).

Table S8. Time-dependent products formation in PhOMe



Time [min]	Products Ratio			
	1b	**3ba**	**4ba**	**5ba**
0	93	7	0	0
15	11	44	44	0
30	2	30	69	0
60	0	11	82	7
120	0	0	84	16

Table S9. Time-dependent products formation in DCM

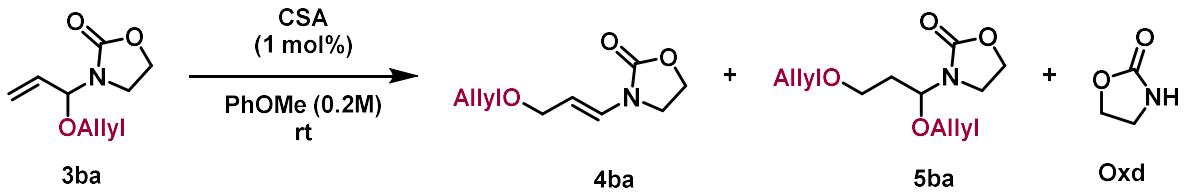


Time [min]	Products Ratio			
	1b	3ba	4ba	5ba
0	95	5	0	0
15	31	45	24	0
30	9	39	52	0
60	3	24	73	0
120	0	9	79	11

4. Interconversion between products **3ba** and **4ba**

We confirmed the CSA-promoted products interconversion subjecting isolated **3ba** to CSA in anisole at room temperature (Table S10). We observed that over time product **3ba** is converted into **4ba**, however, we also observed some reagent degradation, yielding 2-oxazolidinone (Oxd) and free allyl alcohol. The latter adds to product **4ba** providing **5ba**.

Table S10. Interconversion between products **3ba** and **4ba** in anisole at room temperature.[a]

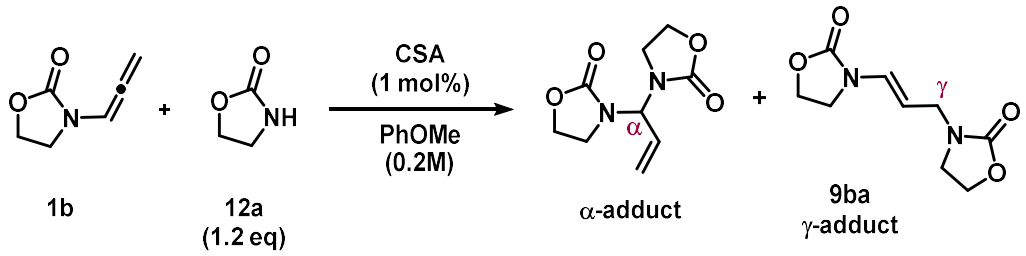


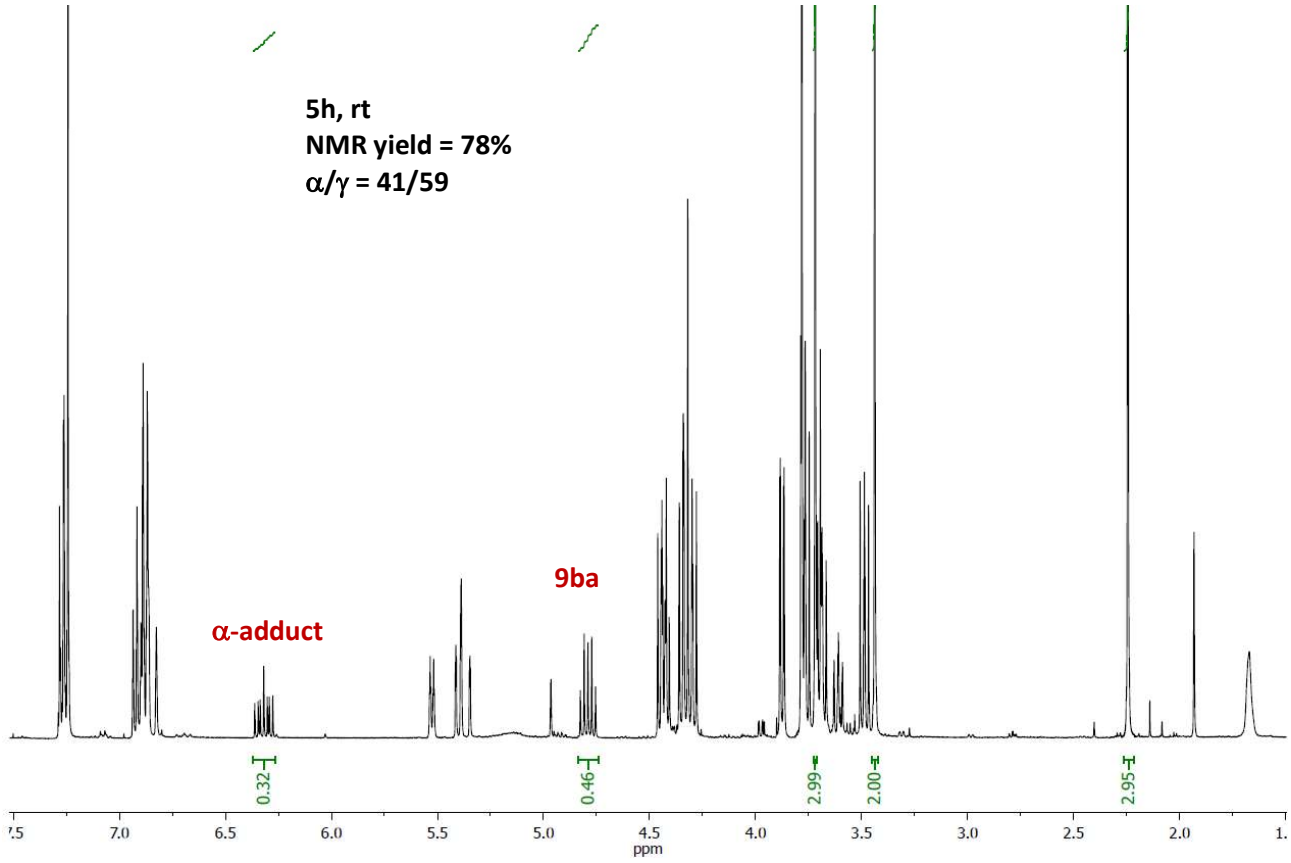
Entry	Time [h]	Conversion [%][b]	Products Yield [%][b]		
			4ba	5ba	Oxd
1	5	94	66	14	14

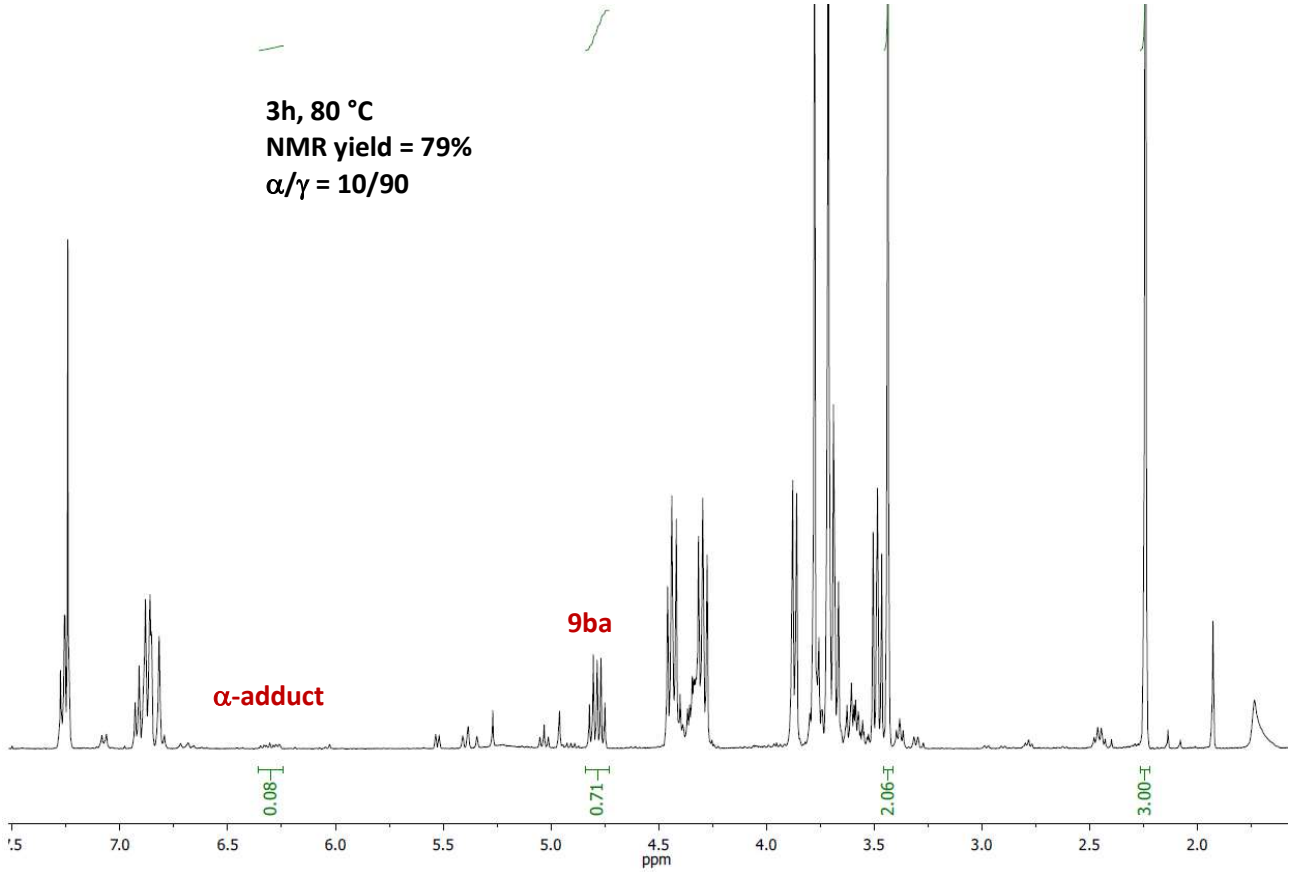
[a] Reaction conditions: **3ba** (0.1 mmol), PhOMe (0.2 M), CSA (1 mol%, stock solution 0.025 M in PhOMe), PhOMe (0.2 M), rt. [b] Conversion and products yield determined by ^{1}H-NMR analysis of the crude using methyl acetoacetate as internal standard.

During the conditions optimization for the amides addition, we monitored the products distribution over the time via ^{1}H NMR (Figure S6), demonstrating that enamide **9ba** derived from the corresponding α-adduct.

Figure S6. ^{1}H-NMR spectra of the reaction mixture related to the addition of oxazolidinone **12a** to allenamide **1b**.




5h, rt
NMR yield = 78%
α/γ = 41/59
9ba
α-adduct
0.32
0.46
2.99
2.00
2.95
ppm

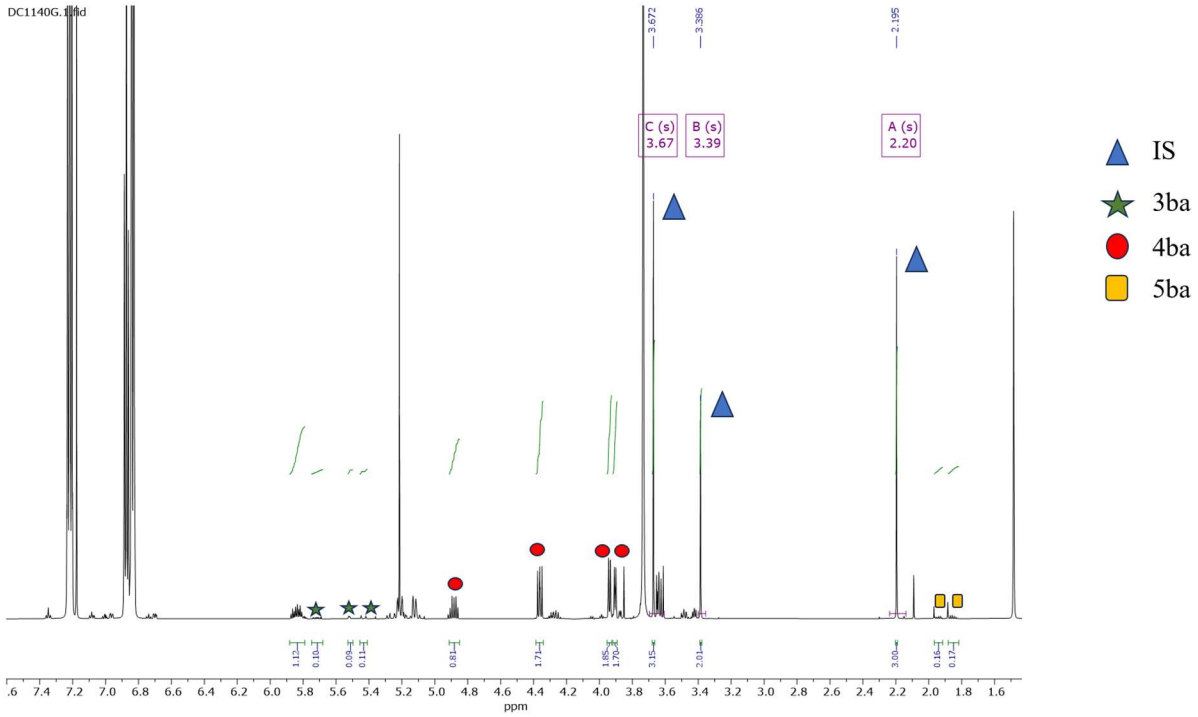

3h, 80 °C
NMR yield = 79%
α/γ = 10/90
9ba
α-adduct
0.08
0.71
2.06
3.00
ppm

4. Products Characterization

1. Use of methyl acetoacetate as internal standard

For the evaluation of NMR yield, after the completion of the reaction, the crude mixture is quenched, dried under *vacuum*, dissolved in 0.3 mL of $CDCl_3$ and 0.1 mmol (10.8 µL, 1 eq.) of methyl acetoacetate is added. This mixture is then transferred in a NMR tube and diluted with $CDCl_3$. After ^{1}H-NMR analysis, we integrate the internal standard (IS) peaks and the characteristic peaks of the products. We determine the NMR yield by comparison between the integrals of the peak at 2.20 ppm of the internal standard and the various products peaks.

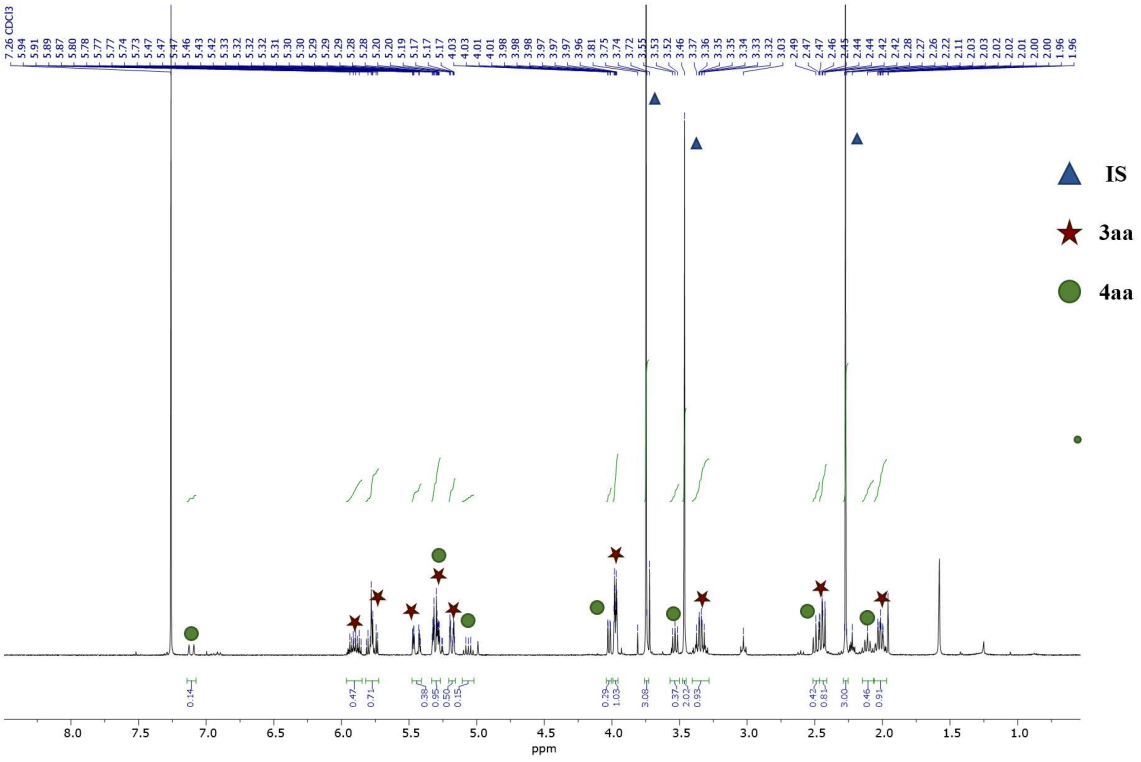
Figure S7. Evaluation of the NMR yield using methyl acetoacetate as internal standard (IS)



2. Characterization of Product **3aa**

Product **3aa** was obtained with a good NMR yield only in the reaction promoted by TFA (Table S2, entry 7), thus it wasn't isolated and fully characterized. Here, in Figure S8, the ^{1}H NMR spectrum of the crude mixture is reported.

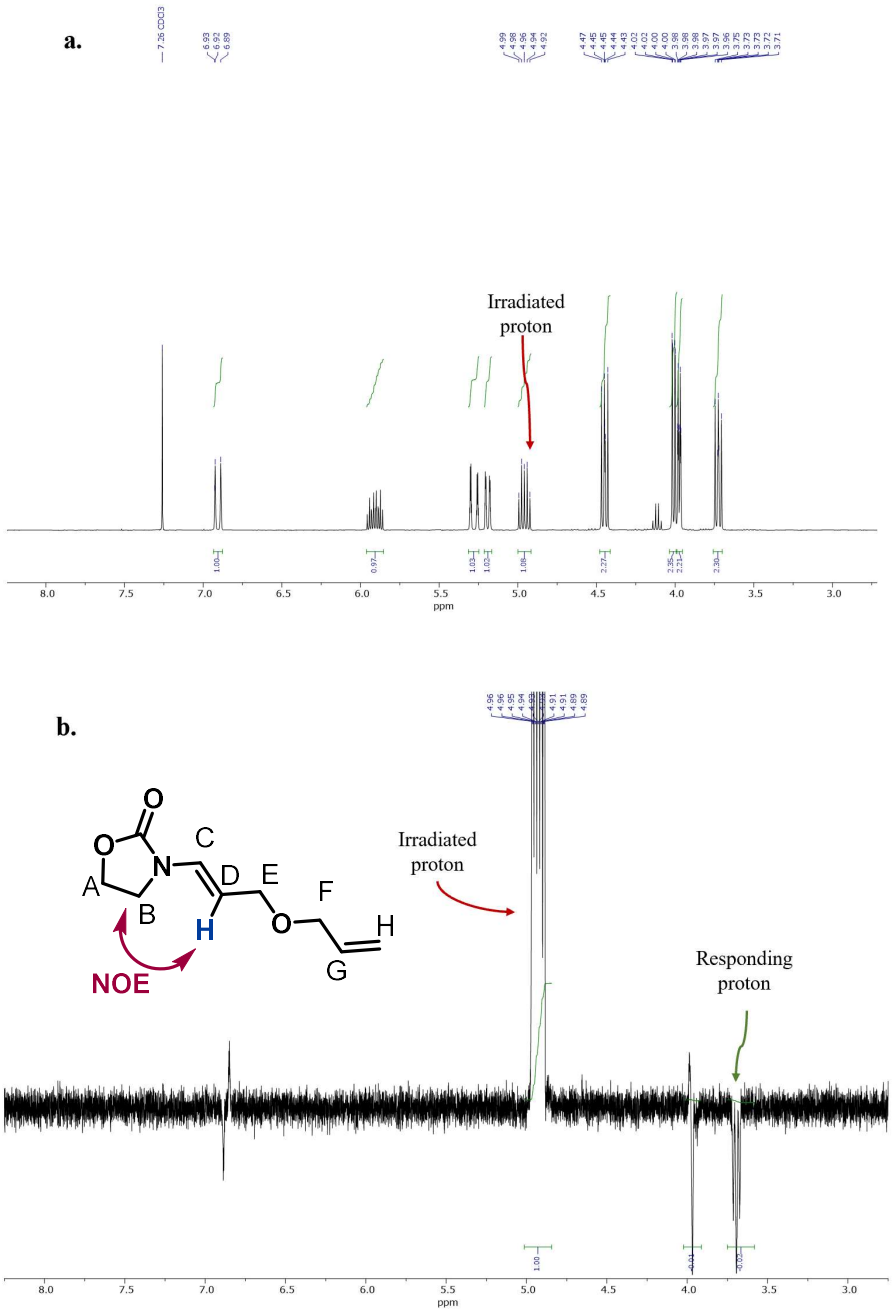
Figure S8. Crude ^{1}H NMR spectrum of product **3aa** (Table S2, entry 7). IS = internal standard (methyl acetoacetate)



3. Stereochemistry determination of the double bond of product **4ba**

In order to confirm the stereochemistry of the double bond in the obtained enamides, a 1D NOESY experiment was performed on the model product **4ba**. As shown in Figure S9, proton **D** (4.96 ppm, dt, J = 14.2, 7.0 Hz, 1H) was irradiated and a NOE effect was observed with proton **B** (3.76 – 3.70, m, 2H), suggesting that proton **D** is facing the oxazolidinone ring and, therefore, the double bond has an *E* configuration.

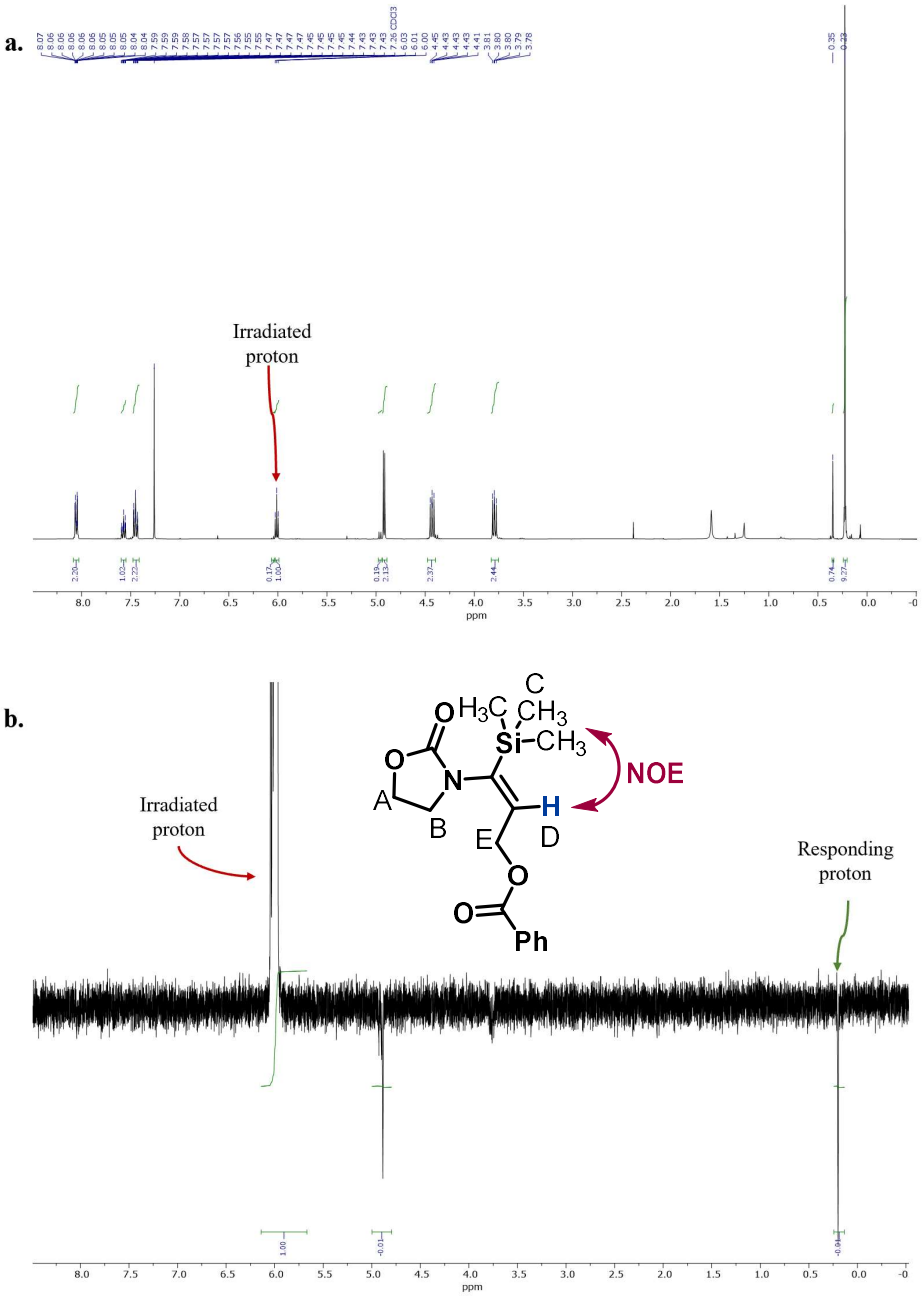
Figure S9. a. ^{1}H NMR spectrum of product **4ba** that shows the irradiated signal. **b.** Recorded 1D NOESY spectrum.



4. Stereochemistry determination of the double bond of product **10gb**

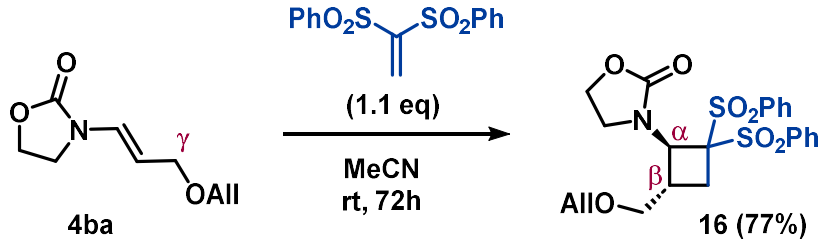
In order to confirm the stereochemistry of the double bond of the major diastereoisomer of products obtained from allenamide **10g** (bearing a further TMS-substituent on the double bond), a 1D NOESY experiment was performed on product **10gb**. As shown in Figure S10, proton **D** (6.01 ppm, t, J = 5.9 Hz, 1H, *major diastereoisomer*) was irradiated and a NOE effect was observed with protons **C** (0.23 ppm, s, 9H, *major diastereoisomer*), suggesting that proton **D** is facing the trimethylsilyl substituent and that the double bond has an *E* configuration.

Figure S10. a. ^{1}H NMR spectrum of product **10gb** that shows the irradiated signal. **b.** 1D NOESY spectrum.



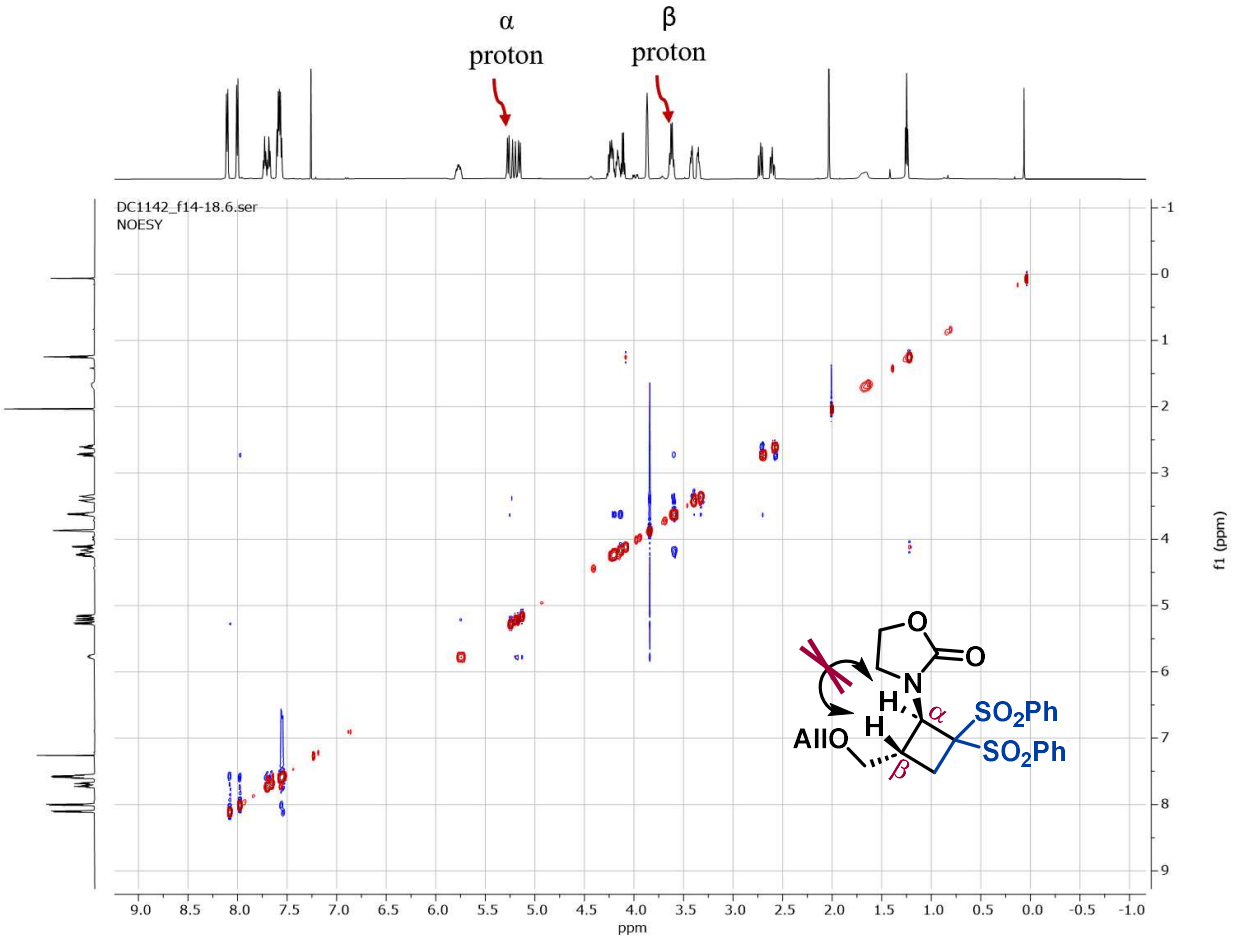
5. Characterization of product **16**

Scheme S1. Synthesis of product **16**



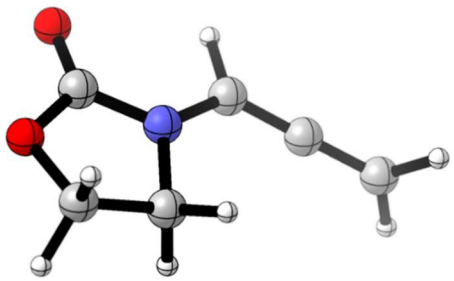
The structure of product **16** was confirmed thanks to ^{1}H – ^{1}H COSY and ^{1}H – ^{13}C HSQC experiments. The corresponding spectra are reported in the following section. The *trans* configuration was determined through a 2D NOESY experiment. Indeed, no correlation between the protons in α and β positions was observed, suggesting that the two protons are facing opposite sides of the cyclobutane ring (Figure S11).

Figure S11. 2D NOESY spectrum of product **16**



5. DFT Calculations

s-trans 1b



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000018	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.001085	0.001800	YES
RMS Displacement	0.000277	0.001200	YES

Predicted change in Energy=-8.512906D-09

Optimization completed.

SCF Done: E(RM062X) = -437.825130337 A.U. after 8 cycles

Zero-point correction=	0.126781 (Hartree/Particle)
Thermal correction to Energy=	0.135089
Thermal correction to Enthalpy=	0.136034
Thermal correction to Gibbs Free Energy=	0.093154
Sum of electronic and zero-point Energies=	-437.698349
Sum of electronic and thermal Energies=	-437.690041
Sum of electronic and thermal Enthalpies=	-437.689097
Sum of electronic and thermal Free Energies=	-437.731976

Eigenvalues --- 0.00151 0.00346 0.00698 0.01223 0.02140

Item	Value	Threshold	Converged?
Maximum Force	0.000018	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.001102	0.001800	YES
RMS Displacement	0.000292	0.001200	YES

Predicted change in Energy=-1.033126D-08

Optimization completed.

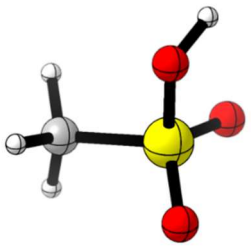
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.257477	0.729916	0.012413
7	0.037932	0.112362	-0.117131
6	0.131911	-1.318994	0.080909
6	1.643300	-1.517713	-0.102490
8	2.216657	-0.219940	0.113832
8	1.479422	1.915185	0.036657
6	-1.161907	0.830740	-0.086721
6	-2.343589	0.266727	-0.012702
6	-3.527973	-0.278824	0.053243
1	-0.456735	-1.860774	-0.663044
1	-0.221404	-1.593508	1.081930
1	1.889105	-1.835479	-1.118438
1	2.080132	-2.208206	0.617253
1	-1.029555	1.907743	-0.133251
1	-4.080994	-0.549222	-0.843977
1	-4.010010	-0.480155	1.007611

Single point calculation:

SCF Done: E(RM062X) = -437.997325661 A.U. after 12 cycles

Corrected Single point: -437.903917

Methanesulfonic acid



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000022	0.000450	YES
RMS Force	0.000008	0.000300	YES
Maximum Displacement	0.000306	0.001800	YES
RMS Displacement	0.000137	0.001200	YES

Predicted change in Energy=-4.834261D-09

Optimization completed.

SCF Done: E(RM062X) = -664.168348728 A.U. after 8 cycles

Zero-point correction=	0.062629 (Hartree/Particle)
Thermal correction to Energy=	0.068517
Thermal correction to Enthalpy=	0.069461
Thermal correction to Gibbs Free Energy=	0.033349
Sum of electronic and zero-point Energies=	-664.105720
Sum of electronic and thermal Energies=	-664.099832
Sum of electronic and thermal Enthalpies=	-664.098888
Sum of electronic and thermal Free Energies=	-664.135000

Eigenvalues --- 0.00045 0.00251 0.04232 0.04338 0.09849

Item	Value	Threshold	Converged?
Maximum Force	0.000022	0.000450	YES
RMS Force	0.000008	0.000300	YES
Maximum Displacement	0.000604	0.001800	YES
RMS Displacement	0.000207	0.001200	YES

Predicted change in Energy=-5.194917D-09

Optimization completed.

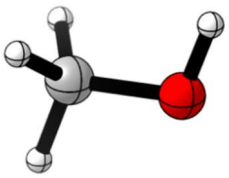
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.622398	-0.332621	0.001885
1	-1.937266	-0.353057	-1.041317
1	-2.182400	0.421676	0.556223
1	-1.731073	-1.312469	0.466131
16	0.086308	0.134948	0.060096
8	0.262069	1.381052	-0.653896
8	0.597285	-0.020749	1.411076
8	0.754492	-1.025630	-0.843310
1	1.293423	-1.596967	-0.264843

Single point calculation:

SCF Done: E(RM062X) = -664.358705311 A.U. after 12 cycles

Corrected Single point: -664.325357

Methanol



--- Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000208	0.000450	YES
RMS Force	0.000107	0.000300	YES
Maximum Displacement	0.001474	0.001800	YES
RMS Displacement	0.000821	0.001200	YES

Predicted change in Energy=-4.571812D-07

Optimization completed.

SCF Done: E(RM062X) = -115.658368172   A.U. after   8 cycles

Zero-point correction=   0.052155 (Hartree/Particle)

Thermal correction to Energy=   0.055435

Thermal correction to Enthalpy=   0.056379

Thermal correction to Gibbs Free Energy=   0.029449

Sum of electronic and zero-point Energies=   -115.606213

Sum of electronic and thermal Energies=   -115.602934

Sum of electronic and thermal Enthalpies=   -115.601989

Sum of electronic and thermal Free Energies=   -115.628919

    Eigenvalues ---   0.00342   0.09198   0.09199   0.13751   0.16289

Item	Value	Threshold	Converged?
Maximum Force	0.000208	0.000450	YES
RMS Force	0.000107	0.000300	YES
Maximum Displacement	0.001215	0.001800	YES
RMS Displacement	0.000706	0.001200	YES

Predicted change in Energy=-4.154643D-07

Optimization completed.

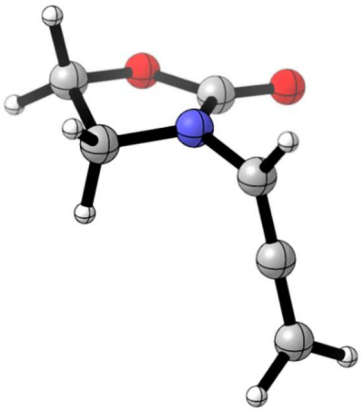
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.661347	-0.019628	0.000000
1	1.084129	0.987078	-0.000001
1	1.024945	-0.546240	-0.891537
1	1.024945	-0.546238	0.891538
8	-0.746327	0.123329	0.000000
1	-1.131480	-0.763462	0.000000

Single point calculation:

SCF Done: E(RM062X) = -115.717365039 A.U. after 9 cycles

Corrected Single point: -115.687916

TS1



-- Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000023	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.000786	0.001800	YES
RMS Displacement	0.000249	0.001200	YES

Predicted change in Energy=-8.826944D-09

Optimization completed.

SCF Done: E(RM062X) = -437.814480463 A.U. after 10 cycles

Zero-point correction= 0.126406 (Hartree/Particle)

Thermal correction to Energy= 0.133859

Thermal correction to Enthalpy= 0.134803

Thermal correction to Gibbs Free Energy= 0.093872

Sum of electronic and zero-point Energies= -437.688074

Sum of electronic and thermal Energies= -437.680621

Sum of electronic and thermal Enthalpies= -437.679677

Sum of electronic and thermal Free Energies= -437.720608

Eigenvalues --- -0.00419 0.00244 0.00413 0.01207 0.02049

Item	Value	Threshold	Converged?
Maximum Force	0.000022	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.000826	0.001800	YES
RMS Displacement	0.000258	0.001200	YES

Predicted change in Energy=-8.960844D-09

Optimization completed.

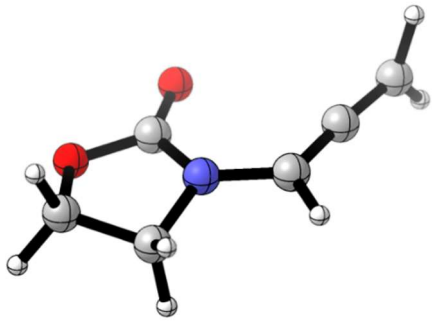
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.787557	0.886961	0.032478
7	-0.135631	-0.202612	0.559504
6	-0.733670	-1.439458	0.077647
6	-2.133031	-0.929325	-0.276918
8	-1.947216	0.467879	-0.537215
8	-0.440608	2.040801	0.051192
6	1.229535	-0.124956	0.968958
6	2.207781	-0.156731	0.098508
6	3.177756	-0.191388	-0.771641
1	-0.751842	-2.206407	0.854254
1	-0.190386	-1.821537	-0.795601
1	-2.824841	-1.036522	0.562922
1	-2.555337	-1.392808	-1.167551
1	1.419980	-0.054485	2.036672
1	3.618324	-1.133290	-1.086840
1	3.571229	0.723272	-1.206397

Single point calculation:

SCF Done: E(RM062X) = -437.986743940 A.U. after 12 cycles

Corrected Single point: -437.892565

s-cis 1b



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000036	0.000450	YES
RMS Force	0.000009	0.000300	YES
Maximum Displacement	0.000825	0.001800	YES
RMS Displacement	0.000295	0.001200	YES

Predicted change in Energy=-1.607861D-08

Optimization completed.

SCF Done: E(RM062X) = -437.818822455 A.U. after 8 cycles

Zero-point correction= 0.126598 (Hartree/Particle)

Thermal correction to Energy= 0.134965

Thermal correction to Enthalpy= 0.135909

Thermal correction to Gibbs Free Energy= 0.092665

Sum of electronic and zero-point Energies= -437.692224

Sum of electronic and thermal Energies= -437.683857

Sum of electronic and thermal Enthalpies= -437.682913

Sum of electronic and thermal Free Energies= -437.726157

Eigenvalues --- 0.00118 0.00220 0.00369 0.01130 0.02178

Item	Value	Threshold	Converged?
Maximum Force	0.000036	0.000450	YES
RMS Force	0.000009	0.000300	YES
Maximum Displacement	0.000565	0.001800	YES
RMS Displacement	0.000168	0.001200	YES

Predicted change in Energy=-2.128935D-08

Optimization completed.

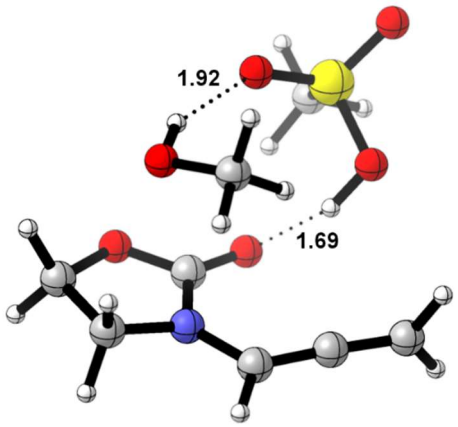
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.480993	0.833556	-0.005506
7	-0.216877	-0.511205	0.086541
6	-1.417052	-1.298509	-0.145922
6	-2.487807	-0.241115	0.141442
8	-1.825819	1.009541	-0.082837
8	0.309670	1.741746	-0.021795
6	1.071295	-1.069550	0.026344
6	2.216202	-0.428985	0.010938
6	3.405627	0.106351	0.005383
1	-1.477973	-2.147517	0.538090
1	-1.453544	-1.662569	-1.179155
1	-2.819178	-0.276245	1.182624
1	-3.347454	-0.300527	-0.524227
1	1.063849	-2.156254	0.010946
1	3.904364	0.373627	-0.923474
1	3.933628	0.327140	0.930392

Single point calculation:

SCF Done: E(RM062X) = -437.991073782 A.U. after 12 cycles

Corrected Single point: -437.897544

I1



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000004	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000414	0.001800	YES
RMS Displacement	0.000090	0.001200	YES

Predicted change in Energy=-7.561593D-10

Optimization completed.

SCF Done: E(RM062X) = -1217.69085137 A.U. after 9 cycles

Zero-point correction= 0.246158 (Hartree/Particle)

Thermal correction to Energy= 0.265569

Thermal correction to Enthalpy= 0.266513

Thermal correction to Gibbs Free Energy= 0.196831

Sum of electronic and zero-point Energies= -1217.444693

Sum of electronic and thermal Energies= -1217.425283

Sum of electronic and thermal Enthalpies= -1217.424339

Sum of electronic and thermal Free Energies= -1217.494021

Eigenvalues --- 0.00041 0.00108 0.00123 0.00197 0.00244

Item	Value	Threshold	Converged?
Maximum Force	0.000004	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000603	0.001800	YES

RMS Displacement 0.000128 0.001200 YES

Predicted change in Energy=-9.297160D-10

Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.288000	-0.278018	-0.955501
7	2.290782	0.385239	-0.331179
6	3.337544	-0.522099	0.113675
6	2.898362	-1.836084	-0.559330
8	1.620844	-1.555471	-1.156159
8	0.225356	0.187325	-1.345636
6	2.259114	1.741766	0.038243
6	1.226304	2.547379	-0.033159
6	0.244077	3.405856	-0.073696
1	3.332199	-0.605829	1.203319
1	4.317126	-0.178791	-0.228276
1	2.757851	-2.637565	0.163273
1	3.574405	-2.150134	-1.355464
1	3.215379	2.109028	0.400856
1	0.044996	4.001724	-0.961717
1	-0.423080	3.540518	0.775052
6	-2.847817	-0.726245	-1.644420
1	-3.456316	0.049943	-2.108299
1	-3.360053	-1.688737	-1.674194
1	-1.862701	-0.792906	-2.108145
16	-2.608815	-0.304629	0.061351
8	-3.882598	-0.043489	0.700250
8	-1.716378	-1.297335	0.651983
8	-1.865934	1.101660	-0.020197
1	-0.964235	0.973201	-0.430902
6	0.636383	-0.202330	2.334243
1	1.587857	0.234628	2.651966
1	0.029938	-0.407030	3.225278
1	0.109155	0.536859	1.717200
8	0.926923	-1.382798	1.611071

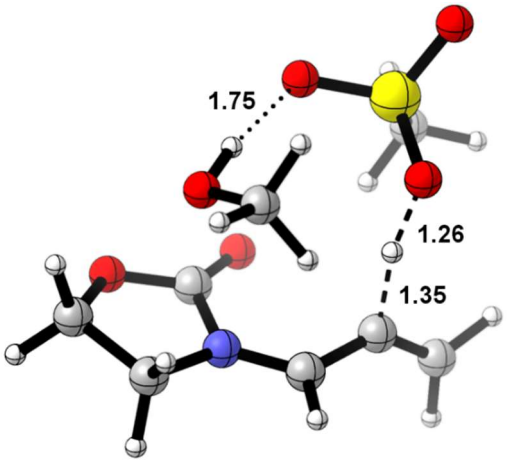
1 0.085526 -1.667989 1.215859

Single point calculation:

SCF Done: E(RM062X) = -1218.10518641 A.U. after 12 cycles

Corrected Single point: -1217.903999

TS2



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000003	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000510	0.001800	YES
RMS Displacement	0.000157	0.001200	YES

Predicted change in Energy=-1.030770D-09

Optimization completed.

SCF Done: E(RM062X) = -1217.65731804 A.U. after 7 cycles

Zero-point correction= 0.242054 (Hartree/Particle)

Thermal correction to Energy= 0.260325

Thermal correction to Enthalpy= 0.261270

Thermal correction to Gibbs Free Energy= 0.195155

Sum of electronic and zero-point Energies= -1217.415264

Sum of electronic and thermal Energies= -1217.396993

Sum of electronic and thermal Enthalpies= -1217.396048

Sum of electronic and thermal Free Energies=   -1217.462163

Eigenvalues ---   -0.04566   0.00119   0.00183   0.00280   0.00330

Item	Value	Threshold	Converged?
Maximum Force	0.000003	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000502	0.001800	YES
RMS Displacement	0.000149	0.001200	YES

Predicted change in Energy=-9.733565D-10

Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.607721	0.344629	1.079628
7	-2.024132	0.721336	-0.232501
6	-3.241269	0.007713	-0.617181
6	-3.471292	-0.903393	0.602528
8	-2.508093	-0.487095	1.583693
8	-0.631187	0.751170	1.635791
6	-1.310780	1.497923	-1.031307
6	-0.016266	1.959582	-0.809040
6	0.571602	3.135099	-0.629715
1	-3.064888	-0.566794	-1.527565
1	-4.053743	0.719584	-0.771800
1	-3.271084	-1.946739	0.369393
1	-4.459857	-0.779542	1.041463
1	-1.755405	1.636973	-2.018225
1	0.016594	4.048840	-0.431046
1	1.655901	3.208871	-0.636069
6	2.645378	0.816772	1.311242
1	3.320280	1.562942	0.890105
1	3.069967	0.390608	2.221069
1	1.658767	1.238321	1.510900
16	2.459124	-0.500868	0.133664
8	3.780556	-1.021581	-0.199470

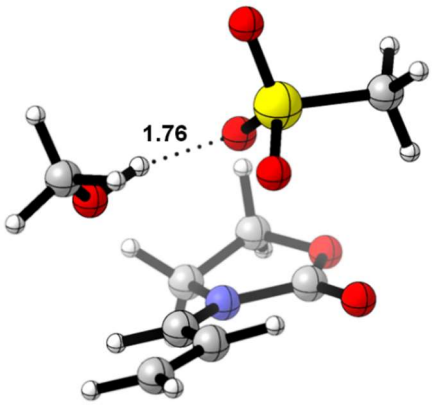
8	1.513147	-1.466866	0.723635
8	1.840397	0.175680	-1.102192
1	0.854928	0.937073	-0.916635
6	-0.585037	-1.792088	-1.805928
1	-1.342621	-2.358179	-2.356474
1	0.393995	-2.250184	-1.979798
1	-0.544081	-0.770855	-2.218107
8	-0.928830	-1.798785	-0.436355
1	-0.091428	-1.723989	0.069484

Single point calculation:

SCF Done: E(RM062X) = -1218.06947273 A.U. after 13 cycles

Corrected Single point: -1217.87117

I2



-- Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000023	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.000985	0.001800	YES
RMS Displacement	0.000276	0.001200	YES

Predicted change in Energy=-4.364336D-09

Optimization completed.

SCF Done: E(RM062X) = -1217.70042695 A.U. after 8 cycles

Zero-point correction= 0.248841 (Hartree/Particle)

Thermal correction to Energy= 0.267447

Thermal correction to Enthalpy= 0.268391

Thermal correction to Gibbs Free Energy= 0.201276

Sum of electronic and zero-point Energies= -1217.451586

Sum of electronic and thermal Energies= -1217.432980

Sum of electronic and thermal Enthalpies= -1217.432036

Sum of electronic and thermal Free Energies= -1217.499151

Eigenvalues --- 0.00087 0.00198 0.00242 0.00286 0.00335

Item	Value	Threshold	Converged?
Maximum Force	0.000023	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.001036	0.001800	YES
RMS Displacement	0.000346	0.001200	YES

Predicted change in Energy=-6.809814D-09

Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.699530	-1.628735	-0.769154
7	1.580630	-0.810321	0.036518
6	1.822382	-1.461106	1.328056
6	0.754152	-2.562600	1.322827
8	0.374689	-2.695315	-0.058769
8	0.405353	-1.416555	-1.905101
6	2.019392	0.380535	-0.263012
6	1.718759	1.136469	-1.447279
6	2.347333	2.315326	-1.579065
1	1.683244	-0.730991	2.125856
1	2.837588	-1.863335	1.345684
1	-0.133563	-2.272194	1.880617
1	1.137540	-3.527127	1.648503
1	2.717061	0.803886	0.451097
1	3.056713	2.668872	-0.834969

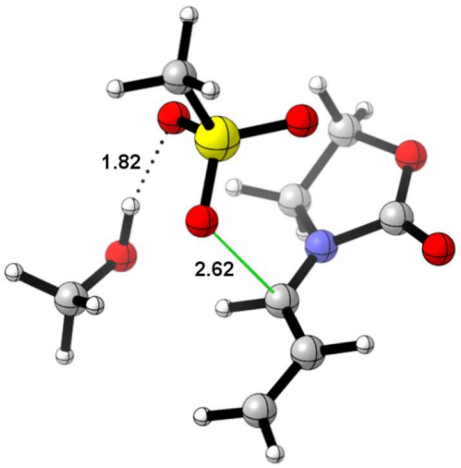
1	2.162384	2.959328	-2.431855
6	-2.804882	-0.934622	-0.911216
1	-3.491737	-0.472460	-1.621508
1	-3.358614	-1.530661	-0.184975
1	-2.074142	-1.549291	-1.438836
16	-1.942379	0.365036	-0.044788
8	-2.958557	1.167599	0.651082
8	-1.036155	-0.366037	0.913075
8	-1.157902	1.100324	-1.057883
1	0.980884	0.773567	-2.147261
6	0.424088	2.790557	1.379368
1	1.322810	3.414747	1.386613
1	-0.276010	3.184253	2.126416
1	-0.045696	2.844940	0.390811
8	0.818136	1.465109	1.691041
1	0.046156	0.872177	1.534079

Single point calculation:

SCF Done: E(RM062X) = -1218.10945832 A.U. after 13 cycles

Corrected Single point: -1217.904627

I4



-- Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000011	0.000450	YES

```
RMS     Force            0.000002     0.000300     YES
Maximum Displacement     0.000692     0.001800     YES
RMS     Displacement     0.000162     0.001200     YES
Predicted change in Energy=-1.682743D-09
Optimization completed.

SCF Done:  E(RM062X) =  -1217.70632945     A.U. after    7 cycles

Zero-point correction=                           0.248583 (Hartree/Particle)
Thermal correction to Energy=                    0.267330
Thermal correction to Enthalpy=                  0.268274
Thermal correction to Gibbs Free Energy=         0.200381
Sum of electronic and zero-point Energies=          -1217.457746
Sum of electronic and thermal Energies=             -1217.439000
Sum of electronic and thermal Enthalpies=           -1217.438056
Sum of electronic and thermal Free Energies=        -1217.505948

    Eigenvalues ---    0.00011    0.00151    0.00190    0.00243    0.00409

         Item               Value     Threshold  Converged?
Maximum Force            0.000011     0.000450     YES
RMS     Force            0.000002     0.000300     YES
Maximum Displacement     0.000765     0.001800     YES
RMS     Displacement     0.000175     0.001200     YES
Predicted change in Energy=-1.859014D-09
Optimization completed.

 Atomic           Coordinates (Angstroms)
 Number         X            Y            Z
---------------------------------------------------------------------
    6         2.402202     0.221542    -0.227800
    7         1.258351     0.748902     0.500787
    6         1.187942     0.102867     1.820189
    6         2.069845    -1.123889     1.596503
    8         2.923987    -0.751452     0.495026
    8         2.819578     0.651492    -1.258362
    6         0.377869     1.592609     0.043161
```

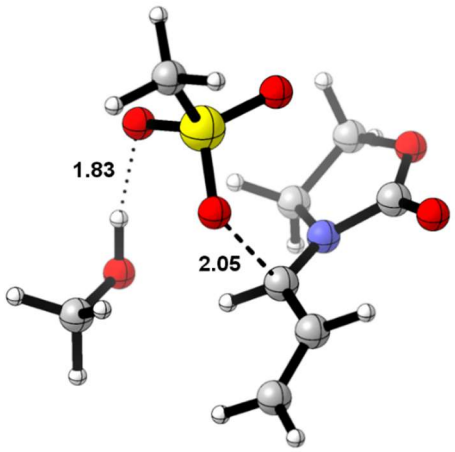
6	0.449963	2.317348	-1.198972
6	-0.505850	3.230425	-1.420906
1	0.158681	-0.153535	2.063353
1	1.607021	0.789080	2.559526
1	1.483693	-1.986904	1.284875
1	2.712972	-1.350212	2.444032
1	-0.463384	1.768837	0.717751
1	-1.307300	3.396777	-0.705738
1	-0.514256	3.830723	-2.324090
6	-1.847132	-2.583665	-1.494383
1	-2.909367	-2.415748	-1.313841
1	-1.555712	-3.578318	-1.155534
1	-1.615131	-2.459081	-2.552492
16	-0.918027	-1.377703	-0.568935
8	-1.274739	-1.598394	0.864668
8	0.512363	-1.645410	-0.843503
8	-1.360657	-0.042893	-1.041744
1	1.253058	2.126066	-1.896448
6	-3.101925	1.510056	1.162175
1	-3.155628	2.552787	1.487725
1	-4.049485	1.022407	1.423928
1	-2.978946	1.474649	0.073018
8	-2.004485	0.909659	1.825471
1	-1.912097	-0.004356	1.479131

Single point calculation:

SCF Done: E(RM062X) = -1218.11523666 A.U. after 13 cycles

Corrected Single point: -1217.910889

TS4



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000001	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.000225	0.001800	YES
RMS Displacement	0.000052	0.001200	YES

Predicted change in Energy=-1.387511D-10

Optimization completed.

SCF Done: E(RM062X) = -1217.70345720 A.U. after 7 cycles

Zero-point correction= 0.248267 (Hartree/Particle)

Thermal correction to Energy= 0.266317

Thermal correction to Enthalpy= 0.267261

Thermal correction to Gibbs Free Energy= 0.201439

Sum of electronic and zero-point Energies= -1217.455190

Sum of electronic and thermal Energies= -1217.437140

Sum of electronic and thermal Enthalpies= -1217.436196

Sum of electronic and thermal Free Energies= -1217.502018

Eigenvalues --- -0.01216 0.00089 0.00131 0.00169 0.00238

Item	Value	Threshold	Converged?
Maximum Force	0.000001	0.000450	YES
RMS Force	0.000000	0.000300	YES

Maximum Displacement 0.000218 0.001800 YES

RMS Displacement 0.000052 0.001200 YES

Predicted change in Energy=-1.357065D-10

Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.358471	0.365798	-0.270441
7	1.206215	0.769638	0.468467
6	1.166703	0.098582	1.771946
6	2.367965	-0.852902	1.675796
8	3.067638	-0.464821	0.481266
8	2.661500	0.741507	-1.365124
6	0.161356	1.417428	-0.033674
6	0.219026	2.293143	-1.197251
6	-0.690356	3.266480	-1.287946
1	0.225098	-0.438746	1.893125
1	1.274577	0.841814	2.563810
1	2.054629	-1.887563	1.551674
1	3.060682	-0.748800	2.509253
1	-0.639770	1.572953	0.687977
1	-1.467033	3.392244	-0.537732
1	-0.681541	3.969993	-2.113448
6	-1.573984	-2.371807	-1.839986
1	-2.621500	-2.079689	-1.915054
1	-1.487456	-3.431091	-1.594543
1	-1.041223	-2.146916	-2.763825
16	-0.822091	-1.445926	-0.522460
8	-1.586556	-1.750870	0.710590
8	0.600270	-1.823382	-0.456052
8	-1.004662	-0.000463	-0.937151
1	0.999174	2.146274	-1.930896
6	-3.210573	1.284781	1.143185
1	-3.319983	2.325719	1.459329
1	-4.157390	0.766493	1.339021
1	-3.013149	1.258123	0.063232

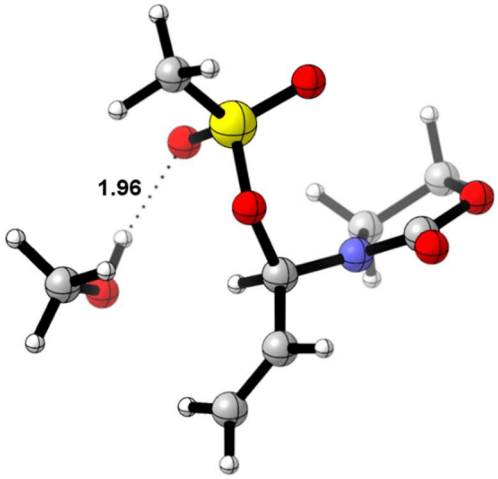
8	-2.141673	0.722691	1.882375
1	-2.038939	-0.199787	1.571162

Single point calculation:

SCF Done: E(RM062X) = -1218.11105378 A.U. after 13 cycles

Corrected Single point: -1217.906432

α-I2



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000004	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.002380	0.001800	NO
RMS Displacement	0.000482	0.001200	YES

Predicted change in Energy=-8.050934D-09

Optimization completed on the basis of negligible forces.

SCF Done: E(RM062X) = -1217.71904488 A.U. after 9 cycles

Zero-point correction=	0.249755 (Hartree/Particle)
Thermal correction to Energy=	0.268108
Thermal correction to Enthalpy=	0.269052
Thermal correction to Gibbs Free Energy=	0.202084
Sum of electronic and zero-point Energies=	-1217.469290
Sum of electronic and thermal Energies=	-1217.450937

Sum of electronic and thermal Enthalpies= -1217.449993

Sum of electronic and thermal Free Energies= -1217.516961

Eigenvalues --- 0.00063 0.00092 0.00220 0.00311 0.00365

Item	Value	Threshold	Converged?
Maximum Force	0.000004	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000726	0.001800	YES
RMS Displacement	0.000127	0.001200	YES

Predicted change in Energy=-6.740644D-10

Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.279660	-0.649314	-0.549373
7	-1.255985	-0.793803	0.362760
6	-1.630249	-0.297439	1.682018
6	-2.992719	0.349309	1.378363
8	-3.353957	-0.123321	0.071989
8	-2.262277	-0.944405	-1.718405
6	0.095041	-0.994034	-0.052873
6	0.336011	-2.227920	-0.868039
6	1.261177	-3.106083	-0.494409
1	-0.907842	0.434232	2.052844
1	-1.705591	-1.122717	2.395434
1	-2.921509	1.437348	1.336076
1	-3.773839	0.048464	2.075125
1	0.734443	-1.001295	0.832723
1	1.865625	-2.940224	0.394963
1	1.442243	-4.012189	-1.063476
6	1.526038	2.421398	-1.428077
1	2.507266	1.948097	-1.462825
1	1.603294	3.460097	-1.103601
1	1.016150	2.352682	-2.388938
16	0.545833	1.580054	-0.220164

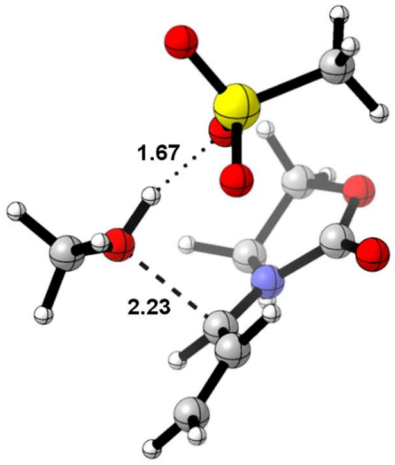
8	1.273692	1.483214	1.045870
8	-0.799069	2.129656	-0.179346
8	0.534555	0.128987	-0.907157
1	-0.282707	-2.354254	-1.750108
6	3.653032	-0.669907	0.281459
1	4.250601	-1.575580	0.155876
1	4.330924	0.192966	0.297659
1	2.983313	-0.582161	-0.585171
8	2.937180	-0.799610	1.496161
1	2.463177	0.038075	1.629409

Single point calculation:

SCF Done: E(RM062X) = -1218.12399981 A.U. after 13 cycles

Corrected Single point: -1217.918044

TS3



-- Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.001010	0.001800	YES
RMS Displacement	0.000163	0.001200	YES

Predicted change in Energy=-1.520207D-09

Optimization completed.

SCF Done: E(RM062X) = -1217.70011555   A.U. after   7 cycles

Zero-point correction=   0.248628 (Hartree/Particle)
Thermal correction to Energy=   0.266220
Thermal correction to Enthalpy=   0.267164
Thermal correction to Gibbs Free Energy=   0.203095
Sum of electronic and zero-point Energies=   -1217.451487
Sum of electronic and thermal Energies=   -1217.433896
Sum of electronic and thermal Enthalpies=   -1217.432952
Sum of electronic and thermal Free Energies=   -1217.497021

    Eigenvalues ---   -0.00271   0.00072   0.00116   0.00175   0.00202

         Item   Value   Threshold Converged?
Maximum Force   0.000006   0.000450   YES
RMS   Force   0.000001   0.000300   YES
Maximum Displacement   0.000972   0.001800   YES
RMS   Displacement   0.000168   0.001200   YES
Predicted change in Energy=-1.610583D-09
Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.618407	1.560853	0.824635
7	1.585473	0.908738	-0.017252
6	1.826865	1.716317	-1.216158
6	0.628225	2.671823	-1.171843
8	0.218755	2.663977	0.207146
8	0.312319	1.222147	1.927887
6	2.069160	-0.303177	0.148546
6	1.761393	-1.181753	1.254109
6	2.585579	-2.216428	1.465940
1	1.824999	1.071848	-2.095543
1	2.782532	2.237304	-1.123047
1	-0.207300	2.304361	-1.765580
1	0.887326	3.695667	-1.431999

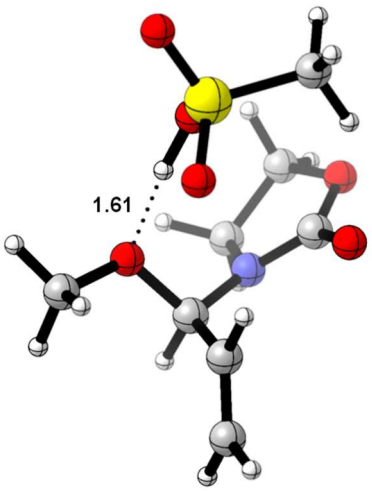
1	2.905201	-0.557891	-0.493679
1	3.463682	-2.385976	0.847393
1	2.407552	-2.919033	2.272766
6	-2.849693	0.788017	0.933734
1	-3.580605	0.299301	1.579387
1	-3.351721	1.465645	0.242231
1	-2.111500	1.322377	1.532911
16	-2.014978	-0.473309	-0.010808
8	-3.039194	-1.170024	-0.801155
8	-1.049297	0.296819	-0.880657
8	-1.288513	-1.322396	0.955086
1	0.864885	-1.005540	1.833540
6	0.709702	-2.662626	-1.365009
1	1.667353	-3.176950	-1.240607
1	0.212218	-3.061204	-2.256225
1	0.083306	-2.840986	-0.485378
8	0.978607	-1.278790	-1.529770
1	0.134170	-0.769164	-1.394513

Single point calculation:

SCF Done: E(RM062X) = -1218.10777272 A.U. after 13 cycles

Corrected Single point: -1217.902281

α-I3



```
 -- Stationary point found.
         Item               Value     Threshold  Converged?
Maximum Force            0.000008     0.000450     YES
RMS     Force            0.000002     0.000300     YES
Maximum Displacement     0.000869     0.001800     YES
RMS     Displacement     0.000287     0.001200     YES
Predicted change in Energy=-3.249004D-09
Optimization completed.

SCF Done:  E(RM062X) =  -1217.73034514     A.U. after    6 cycles

Zero-point correction=                           0.249617 (Hartree/Particle)
Thermal correction to Energy=                    0.267377
Thermal correction to Enthalpy=                  0.268322
Thermal correction to Gibbs Free Energy=         0.202717
Sum of electronic and zero-point Energies=          -1217.480728
Sum of electronic and thermal Energies=             -1217.462968
Sum of electronic and thermal Enthalpies=           -1217.462024
Sum of electronic and thermal Free Energies=        -1217.527628

    Eigenvalues ---    0.00106   0.00174   0.00222   0.00351   0.00376

         Item               Value     Threshold  Converged?
Maximum Force            0.000008     0.000450     YES
RMS     Force            0.000002     0.000300     YES
Maximum Displacement     0.000567     0.001800     YES
RMS     Displacement     0.000221     0.001200     YES
Predicted change in Energy=-2.894631D-09
Optimization completed.

 Atomic          Coordinates (Angstroms)
 Number         X            Y            Z
---------------------------------------------------------------------
   6         0.927856     1.316096     0.826087
   7         1.707187     0.668708    -0.101408
   6         2.051291     1.543560    -1.216252
   6         1.149270     2.754084    -0.932030
```

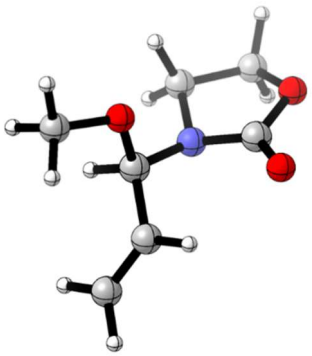
8	0.742760	2.594981	0.433895
8	0.473694	0.881064	1.858634
6	1.826008	-0.756821	-0.236326
6	1.654170	-1.529418	1.042348
6	2.660376	-2.217422	1.570293
1	1.811556	1.069354	-2.170408
1	3.116252	1.794244	-1.193726
1	0.251842	2.748553	-1.554923
1	1.664280	3.708888	-1.025950
1	2.814126	-0.970874	-0.667463
1	3.648399	-2.224410	1.115516
1	2.536268	-2.790511	2.483116
6	-2.649368	0.962095	1.179810
1	-3.425750	0.583322	1.846116
1	-3.003699	1.845026	0.646944
1	-1.723168	1.163758	1.719691
16	-2.328263	-0.305681	-0.013199
8	-3.530130	-0.534389	-0.797251
8	-1.241085	0.421603	-0.931830
8	-1.676610	-1.449157	0.615825
1	0.659743	-1.520469	1.476856
6	0.766252	-2.519093	-1.500789
1	1.759476	-2.904148	-1.756933
1	0.100281	-2.622351	-2.357289
1	0.363654	-3.069183	-0.646775
8	0.842904	-1.125954	-1.218249
1	-0.478745	-0.224906	-1.080765

Single point calculation:

SCF Done: E(RM062X) = -1218.13534221 A.U. after 12 cycles

Corrected Single point: -1217.928965

α-3



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.000518	0.001800	YES
RMS Displacement	0.000140	0.001200	YES

Predicted change in Energy=-1.319888D-09

Optimization completed.

SCF Done: E(RM062X) = -553.537655975 A.U. after 7 cycles

Zero-point correction= 0.184707 (Hartree/Particle)

Thermal correction to Energy= 0.195711

Thermal correction to Enthalpy= 0.196655

Thermal correction to Gibbs Free Energy= 0.147005

Sum of electronic and zero-point Energies= -553.352949

Sum of electronic and thermal Energies= -553.341945

Sum of electronic and thermal Enthalpies= -553.341001

Sum of electronic and thermal Free Energies= -553.390651

Eigenvalues --- 0.00144 0.00308 0.00382 0.00488 0.00745

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.000601	0.001800	YES
RMS Displacement	0.000154	0.001200	YES

Predicted change in Energy=-1.399973D-09

Optimization completed.

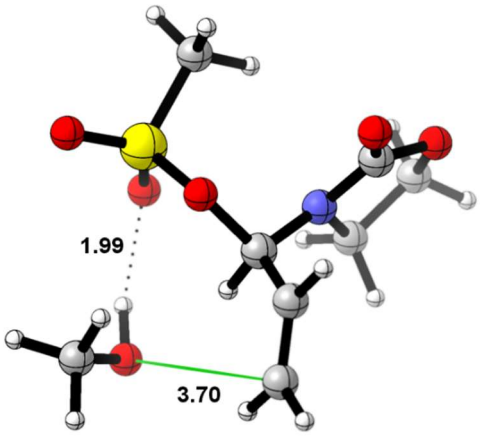
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.218556	0.718324	-0.517192
7	0.530853	0.012413	0.452538
6	1.361577	-1.093613	0.915614
6	2.749774	-0.525973	0.625208
8	2.529932	0.380190	-0.463033
8	0.791064	1.530175	-1.299273
6	-0.894770	-0.198375	0.348353
6	-1.681530	1.081700	0.232255
6	-2.599620	1.422090	1.130632
1	1.153568	-2.001930	0.338236
1	1.203122	-1.290678	1.977859
1	3.474742	-1.274871	0.309458
1	3.142274	0.039852	1.474473
1	-1.198385	-0.714904	1.273204
1	-2.801001	0.801251	2.001231
1	-3.180128	2.334064	1.034452
1	-1.478056	1.689896	-0.642728
6	-2.407518	-1.605601	-0.793515
1	-2.631142	-2.152601	0.133525
1	-2.433802	-2.298993	-1.634747
1	-3.169741	-0.830886	-0.935475
8	-1.105526	-1.057665	-0.755866

Single point calculation:

SCF Done: E(RM062X) = -553.756748202 A.U. after 12 cycles

Corrected Single point: -553.607644

α-I2'



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000019	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.001080	0.001800	YES
RMS Displacement	0.000204	0.001200	YES

Predicted change in Energy=-6.963984D-09

Optimization completed.

SCF Done: E(RM062X) = -1217.71793859 A.U. after 6 cycles

Zero-point correction= 0.249595 (Hartree/Particle)

Thermal correction to Energy= 0.268152

Thermal correction to Enthalpy= 0.269096

Thermal correction to Gibbs Free Energy= 0.200432

Sum of electronic and zero-point Energies= -1217.468343

Sum of electronic and thermal Energies= -1217.449787

Sum of electronic and thermal Enthalpies= -1217.448843

Sum of electronic and thermal Free Energies= -1217.517507

Eigenvalues --- 0.00068 0.00098 0.00166 0.00216 0.00353

Item	Value	Threshold	Converged?
Maximum Force	0.000019	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.001531	0.001800	YES

RMS Displacement 0.000407 0.001200 YES

Predicted change in Energy=-1.492434D-08

Optimization completed.

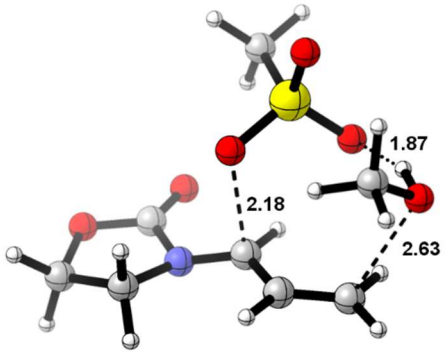
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.351769	0.035718	0.551231
7	1.271428	-0.323592	-0.228044
6	1.716172	-0.817077	-1.523615
6	3.091859	-0.146532	-1.598696
8	3.455520	0.085079	-0.227952
8	2.347611	0.298924	1.727602
6	0.030298	-0.774001	0.356023
8	-0.629619	0.337319	1.010950
16	-1.200024	1.528790	0.084046
8	-1.330771	1.031973	-1.283803
8	-2.364519	2.036843	0.775279
6	0.105277	2.726574	0.151145
6	0.169527	-1.854897	1.384572
6	-0.404855	-3.037858	1.188583
1	1.785437	-1.911416	-1.525504
1	1.043286	-0.491689	-2.319568
1	3.858382	-0.770051	-2.055592
1	3.043212	0.819204	-2.108880
1	-0.601125	-1.124395	-0.463472
1	0.343332	2.906365	1.199752
1	0.963568	2.324130	-0.385637
1	-0.265464	3.634274	-0.327235
1	0.768012	-1.625980	2.261015
1	-1.003889	-3.230025	0.300474
1	-0.300457	-3.846027	1.905099
6	-3.364282	-1.428063	-0.315778
1	-3.730066	-2.424174	-0.057776
1	-2.815883	-1.030969	0.550179
1	-4.225228	-0.777863	-0.510577
8	-2.536657	-1.565418	-1.458582
1	-2.269848	-0.667838	-1.719452

Single point calculation:

SCF Done: E(RM062X) = -1218.12383029 A.U. after 13 cycles

Corrected Single point: -1217.918917

TS5



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000011	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.000457	0.001800	YES
RMS Displacement	0.000160	0.001200	YES

Predicted change in Energy=-1.726688D-09

Optimization completed.

SCF Done: E(RM062X) = -1217.69762294 A.U. after 9 cycles

Zero-point correction= 0.248300 (Hartree/Particle)

Thermal correction to Energy= 0.266205

Thermal correction to Enthalpy= 0.267149

Thermal correction to Gibbs Free Energy= 0.201634

Sum of electronic and zero-point Energies= -1217.449323

Sum of electronic and thermal Energies= -1217.431418

Sum of electronic and thermal Enthalpies= -1217.430474

Sum of electronic and thermal Free Energies= -1217.495989

Eigenvalues --- -0.01138 0.00101 0.00207 0.00257 0.00320

Item	Value	Threshold	Converged?
Maximum Force	0.000011	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.000425	0.001800	YES
RMS Displacement	0.000157	0.001200	YES

Predicted change in Energy=-1.617421D-09

Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.579897	0.454541	-0.518635
7	-1.889805	-0.760352	-0.238702
6	-2.490400	-1.428492	0.912202
6	-3.860162	-0.739064	0.953837
8	-3.676830	0.493082	0.230835
8	-2.218221	1.288365	-1.294282
6	-0.652498	-0.918003	-0.680845
8	0.176992	0.508340	0.750893
16	1.302935	1.343872	0.199724
8	1.793743	0.771832	-1.084114
8	2.355869	1.599987	1.187197
6	0.564369	2.910887	-0.214659
6	0.122479	-2.091684	-0.413863
6	1.181063	-2.349130	-1.201795
1	-1.885506	-1.217330	1.798604
1	-2.569602	-2.503672	0.751629
1	-4.183155	-0.489363	1.961923
1	-4.630021	-1.317181	0.440795
1	-0.347764	-0.243122	-1.475848
1	0.180239	3.361555	0.701257
1	-0.247127	2.735873	-0.921944
1	1.334965	3.544339	-0.655285
1	-0.170675	-2.756099	0.392280
1	1.461547	-1.671417	-2.000596
1	1.770589	-3.250152	-1.085398
6	3.316173	-1.461685	1.054891
1	3.657669	-2.457918	1.350139

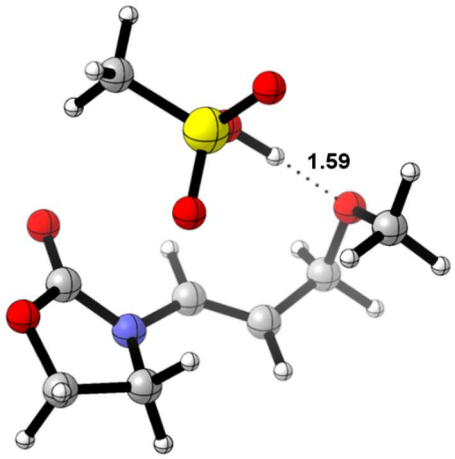
1	2.269226	-1.339295	1.366731
1	3.912533	-0.709561	1.583482
8	3.463111	-1.363741	-0.347598
1	3.064676	-0.513295	-0.622693

Single point calculation:

SCF Done: E(RM062X) = -1218.10729739 A.U. after 13 cycles

Corrected Single point: -1217.90333

γ-I3



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000030	0.000450	YES
RMS Force	0.000006	0.000300	YES
Maximum Displacement	0.001215	0.001800	YES
RMS Displacement	0.000287	0.001200	YES

Predicted change in Energy=-1.000485D-08

Optimization completed.

SCF Done: E(RM062X) = -1217.74019247 A.U. after 7 cycles

Zero-point correction=	0.250933 (Hartree/Particle)
Thermal correction to Energy=	0.268094
Thermal correction to Enthalpy=	0.269038
Thermal correction to Gibbs Free Energy=	0.205548

Sum of electronic and zero-point Energies= -1217.489260

Sum of electronic and thermal Energies= -1217.472098

Sum of electronic and thermal Enthalpies= -1217.471154

Sum of electronic and thermal Free Energies= -1217.534644

Eigenvalues --- 0.00211 0.00234 0.00282 0.00443 0.00581

Item	Value	Threshold	Converged?
Maximum Force	0.000030	0.000450	YES
RMS Force	0.000006	0.000300	YES
Maximum Displacement	0.001346	0.001800	YES
RMS Displacement	0.000321	0.001200	YES

Predicted change in Energy=-1.012456D-08

Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.239332	-0.143742	0.701571
7	-1.715059	1.078177	0.312623
6	-2.115886	1.379352	-1.050461
6	-3.363619	0.498934	-1.172214
8	-3.182805	-0.521565	-0.178832
8	-1.927651	-0.791529	1.671292
6	-0.492489	1.473517	0.830432
8	0.009099	-0.867250	-0.973150
16	1.037750	-1.627707	-0.267612
8	1.530355	-0.833530	1.015225
8	2.195017	-2.053259	-1.043878
6	0.286624	-3.004256	0.550624
6	0.349849	2.328911	0.243163
6	1.733231	2.499030	0.795096
1	-1.318364	1.079275	-1.740216
1	-2.339374	2.440535	-1.177599
1	-3.458848	0.015269	-2.142916
1	-4.278077	1.047894	-0.935777
1	-0.247906	0.968998	1.761454
1	-0.092763	-3.667460	-0.227877

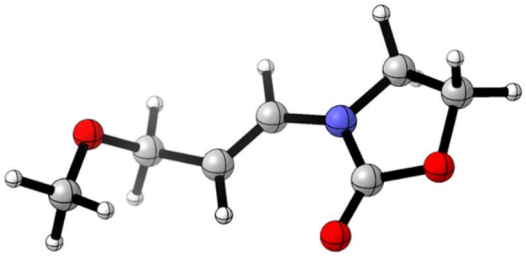
1	-0.528204	-2.617438	1.165204
1	1.043815	-3.507293	1.151531
1	0.096606	2.808092	-0.698172
1	1.738162	2.431020	1.885530
1	2.178135	3.456268	0.500847
6	2.832796	1.423007	-1.042562
1	3.224737	2.388860	-1.380120
1	1.900545	1.193283	-1.571712
1	3.562079	0.636311	-1.238307
8	2.624221	1.448936	0.365778
1	1.987944	0.039516	0.756167

Single point calculation:

SCF Done: E(RM062X) = -1218.14560227 A.U. after 13 cycles

Corrected Single point: -1217.938128

s-cis-4



-- Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000182	0.001800	YES
RMS Displacement	0.000062	0.001200	YES

Predicted change in Energy=-2.109721D-10

Optimization completed.

SCF Done: E(RM062X) = -553.536368594 A.U. after 6 cycles

Zero-point correction= 0.185346 (Hartree/Particle)

Thermal correction to Energy= 0.196454

Thermal correction to Enthalpy= 0.197398

Thermal correction to Gibbs Free Energy= 0.146655

Sum of electronic and zero-point Energies= -553.351022

Sum of electronic and thermal Energies= -553.339914

Sum of electronic and thermal Enthalpies= -553.338970

Sum of electronic and thermal Free Energies= -553.389714

Eigenvalues --- 0.00157 0.00209 0.00274 0.00422 0.00428

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000280	0.001800	YES
RMS Displacement	0.000082	0.001200	YES

Predicted change in Energy=-2.678794D-10

Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.584431	0.871770	-0.128131
7	-1.139599	-0.422758	0.007550
6	-2.258514	-1.351632	0.085599
6	-3.387396	-0.391654	0.471140
8	-2.931517	0.891850	0.026028
8	-0.934695	1.863146	-0.351187
6	0.176724	-0.854518	-0.185093
6	1.254137	-0.106528	-0.435869
6	2.601166	-0.752032	-0.605980
1	-2.086871	-2.117475	0.844510
1	-2.431573	-1.833857	-0.882771
1	-3.532365	-0.350629	1.553731
1	-4.332806	-0.611389	-0.022225
1	0.265574	-1.935221	-0.097639
1	2.492716	-1.839848	-0.658262
1	3.063299	-0.411222	-1.546743
1	1.166336	0.969408	-0.527142
6	3.905022	0.838458	0.541215

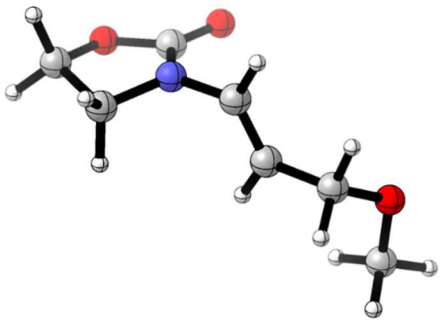
1	4.322036	1.183079	-0.416701
1	4.679486	0.898591	1.308158
1	3.078375	1.504025	0.821681
8	3.497804	-0.507414	0.464317

Single point calculation:

SCF Done: E(RM062X) = -553.756425735 A.U. after 12 cycles

Corrected Single point: -553.607819

TS6



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000002	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.000469	0.001800	YES
RMS Displacement	0.000168	0.001200	YES

Predicted change in Energy=-7.278879D-10

Optimization completed.

SCF Done: E(RM062X) = -553.526725184 A.U. after 8 cycles

Zero-point correction=	0.184606 (Hartree/Particle)
Thermal correction to Energy=	0.195097
Thermal correction to Enthalpy=	0.196042
Thermal correction to Gibbs Free Energy=	0.146862
Sum of electronic and zero-point Energies=	-553.342120
Sum of electronic and thermal Energies=	-553.331628
Sum of electronic and thermal Enthalpies=	-553.330684

Sum of electronic and thermal Free Energies=   -553.379863

Eigenvalues ---   -0.00609   0.00143   0.00191   0.00348   0.00373

Item	Value	Threshold	Converged?
Maximum Force	0.000002	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.000468	0.001800	YES
RMS Displacement	0.000167	0.001200	YES

Predicted change in Energy=-7.237703D-10

Optimization completed.

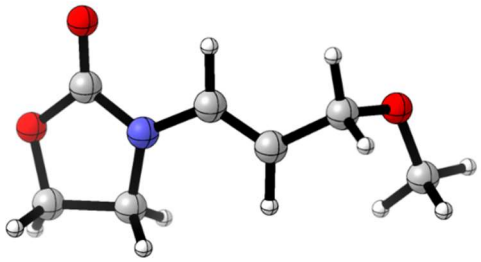
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.721803	0.901171	-0.176917
7	1.175360	-0.333246	-0.414998
6	1.899153	-1.374286	0.298853
6	3.234042	-0.656467	0.526502
8	2.907794	0.737101	0.468120
8	1.274554	1.981794	-0.469557
6	-0.158832	-0.497878	-0.883509
6	-1.207705	-0.483834	-0.067639
6	-2.611739	-0.722982	-0.552101
1	2.008947	-2.275758	-0.307517
1	1.393638	-1.633427	1.237303
1	3.950325	-0.878542	-0.269129
1	3.681914	-0.866051	1.497064
1	-0.268498	-0.663759	-1.954026
1	-2.609308	-0.849442	-1.638664
1	-3.005908	-1.649171	-0.102874
1	-1.050522	-0.309160	0.995996
6	-3.867936	0.424238	1.079463
1	-4.309525	-0.523839	1.418465
1	-4.615603	1.214986	1.158610
1	-3.024674	0.673841	1.736275
8	-3.486225	0.350264	-0.275369

Single point calculation:

SCF Done: E(RM062X) = -553.746737168 A.U. after 12 cycles

Corrected Single point: -553.598436

s-trans-4



-- Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000828	0.001800	YES
RMS Displacement	0.000193	0.001200	YES

Predicted change in Energy=-9.592227D-10

Optimization completed.

SCF Done: E(RM062X) = -553.541078425 A.U. after 8 cycles

Zero-point correction= 0.185306 (Hartree/Particle)

Thermal correction to Energy= 0.196405

Thermal correction to Enthalpy= 0.197349

Thermal correction to Gibbs Free Energy= 0.146599

Sum of electronic and zero-point Energies= -553.355772

Sum of electronic and thermal Energies= -553.344674

Sum of electronic and thermal Enthalpies= -553.343730

Sum of electronic and thermal Free Energies= -553.394480

Eigenvalues --- 0.00118 0.00139 0.00350 0.00448 0.00743

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES

RMS	Force	0.000001	0.000300	YES
Maximum	Displacement	0.000778	0.001800	YES
RMS	Displacement	0.000190	0.001200	YES

Predicted change in Energy=-1.119168D-09

Optimization completed.

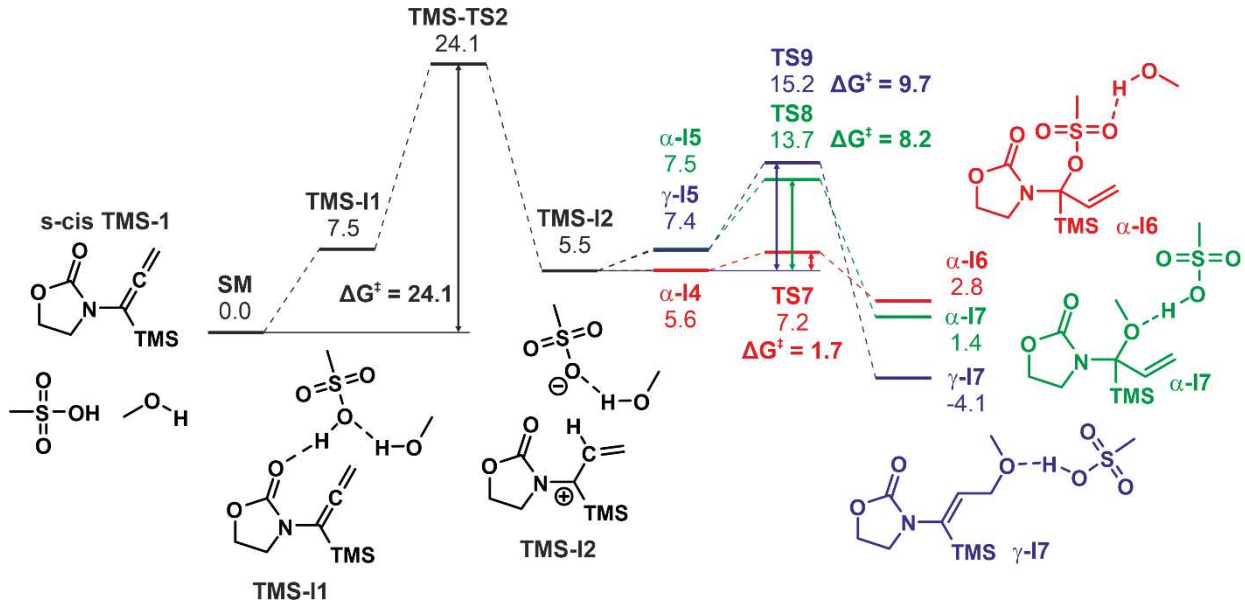
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.160268	0.760318	-0.172459
7	-1.051189	0.030337	0.196432
6	-1.300826	-1.395450	0.143310
6	-2.835330	-1.409745	0.062844
8	-3.201623	-0.083796	-0.343221
8	-2.228889	1.952869	-0.330493
6	0.205428	0.607939	0.317748
6	1.336836	-0.069815	0.527106
6	2.657156	0.636323	0.657567
1	-0.929824	-1.896331	1.041086
1	-0.819082	-1.837965	-0.736383
1	-3.290674	-1.607114	1.035725
1	-3.221415	-2.111510	-0.674863
1	0.180430	1.690833	0.230384
1	2.492609	1.714451	0.740632
1	3.175977	0.300039	1.569797
1	1.320042	-1.153748	0.615898
6	3.990270	-0.855742	-0.583734
1	4.463056	-1.203150	0.347048
1	4.734437	-0.857260	-1.382242
1	3.187585	-1.556330	-0.850339
8	3.518711	0.463772	-0.454545

Single point calculation:

SCF Done: E(RM062X) = -553.761492052 A.U. after 12 cycles

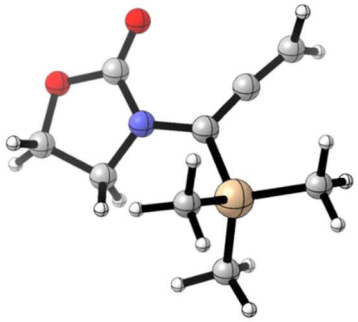
Corrected Single point: -553.613032

Overall reaction profiles for the methanol addition to allenamide s-cis TMS-1



The results on allenamide **1g** show once again that: i. the α-addition of sulfonate anion is the reversible kinetically favored pathway, ii. the addition of methanol in the γ-addition is kinetically unfavored, but it forms the most thermodynamically stable adduct, and iii. the α-addition of methanol is slightly kinetically favored, but potentially reversible.

s-cis TMS-1



-- Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000014	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.001399	0.001800	YES
RMS Displacement	0.000277	0.001200	YES

Predicted change in Energy=-6.223411D-09

Optimization completed.

SCF Done: E(RM062X) = -846.394050148 A.U. after 8 cycles

Zero-point correction=	0.229395 (Hartree/Particle)
Thermal correction to Energy=	0.245450
Thermal correction to Enthalpy=	0.246395
Thermal correction to Gibbs Free Energy=	0.185873
Sum of electronic and zero-point Energies=	-846.164655
Sum of electronic and thermal Energies=	-846.148600
Sum of electronic and thermal Enthalpies=	-846.147656
Sum of electronic and thermal Free Energies=	-846.208177

Eigenvalues --- 0.00062 0.00077 0.00137 0.00211 0.00317

Item	Value	Threshold	Converged?
Maximum Force	0.000014	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.001304	0.001800	YES
RMS Displacement	0.000301	0.001200	YES

Predicted change in Energy=-1.113315D-08

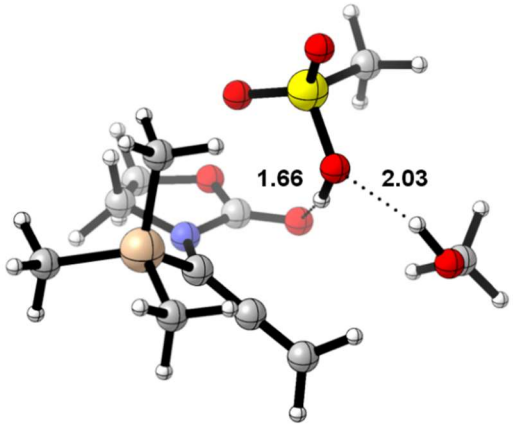
Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.233674	0.591981	-0.163538
7	1.049099	-0.087817	0.004984
6	1.297405	-1.439696	0.482863
6	2.760168	-1.615096	0.066234
8	3.267181	-0.280829	-0.030773
8	2.391219	1.762798	-0.397536
6	-0.216733	0.544726	0.105999
6	-0.371722	1.844930	0.235504
6	-0.676795	3.111184	0.339282
1	0.648112	-2.170757	-0.004149
1	1.156678	-1.503956	1.568720
1	2.844666	-2.091255	-0.914373
1	3.356689	-2.160692	0.795959
1	-0.802546	3.584580	1.309863
1	-0.784287	3.741976	-0.539787
14	-1.808426	-0.483589	-0.080498
6	-2.009401	-1.669890	1.369485
1	-2.997358	-2.140995	1.316929
1	-1.263125	-2.469357	1.380967
1	-1.947075	-1.132998	2.321576
6	-1.712117	-1.426138	-1.706811
1	-0.851265	-2.100466	-1.754453
1	-2.615670	-2.029161	-1.847621
1	-1.637106	-0.728847	-2.547207
6	-3.257080	0.706065	-0.103056
1	-3.315968	1.279786	0.826586
1	-3.177404	1.416224	-0.931299
1	-4.191657	0.146744	-0.218923

Single point calculation:

SCF Done: E(RM062X) = -846.647468446 A.U. after 12 cycles

TMS-I1



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000019	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.000876	0.001800	YES
RMS Displacement	0.000158	0.001200	YES

Predicted change in Energy=-5.975770D-09

Optimization completed.

SCF Done: E(RM062X) = -1626.26260848 A.U. after 6 cycles

Zero-point correction= 0.349416 (Hartree/Particle)

Thermal correction to Energy= 0.376178

Thermal correction to Enthalpy= 0.377122

Thermal correction to Gibbs Free Energy= 0.291823

Sum of electronic and zero-point Energies= -1625.913193

Sum of electronic and thermal Energies= -1625.886431

Sum of electronic and thermal Enthalpies= -1625.885487

Sum of electronic and thermal Free Energies= -1625.970785

Eigenvalues --- 0.00098 0.00136 0.00146 0.00149 0.00167

Item	Value	Threshold	Converged?
Maximum Force	0.000019	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.001090	0.001800	YES

RMS Displacement 0.000216 0.001200 YES

Predicted change in Energy=-1.603672D-08

Optimization completed.

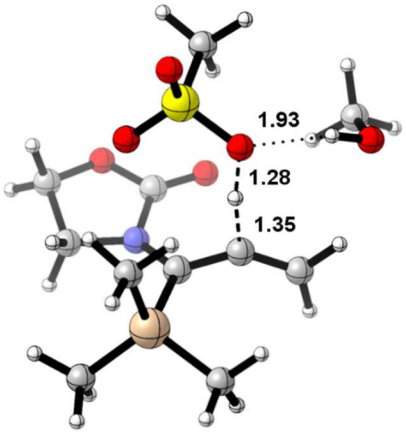
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.112688	-1.401349	-1.472964
7	1.103774	-0.907223	-1.130960
6	1.974416	-1.993739	-0.701947
6	1.282885	-3.181665	-1.376999
8	-0.066984	-2.733885	-1.588556
8	-1.151498	-0.772898	-1.653115
6	1.337206	0.458656	-0.798317
6	0.723931	1.426796	-1.444982
6	0.129977	2.457486	-1.984670
1	1.967419	-2.076722	0.391662
1	2.995437	-1.851427	-1.058893
1	1.249684	-4.076505	-0.758412
1	1.721025	-3.411522	-2.350802
1	0.563918	2.969621	-2.840348
1	-0.819975	2.828008	-1.595821
6	-3.197279	-1.500943	0.911768
1	-4.037158	-0.819211	1.045390
1	-3.340107	-2.410778	1.496074
1	-3.039028	-1.737239	-0.142300
16	-1.726343	-0.704839	1.504571
8	-1.929994	-0.189009	2.842484
8	-0.590988	-1.575975	1.229150
8	-1.635183	0.579073	0.549049
1	-1.365862	0.266204	-0.369988
6	-3.424617	1.917607	-1.572748
1	-3.908218	2.489369	-2.367527
1	-4.178715	1.272874	-1.103023
1	-2.651737	1.281866	-2.026108
8	-2.881693	2.851135	-0.657202
1	-2.525197	2.342482	0.088188
14	2.452437	0.984926	0.660125

6	1.680739	0.472588	2.292695
1	2.324274	0.799991	3.117405
1	0.697959	0.937714	2.423285
1	1.543448	-0.609417	2.370152
6	4.170185	0.226024	0.488302
1	4.857576	0.754925	1.158074
1	4.194256	-0.832057	0.765197
1	4.557633	0.326160	-0.530824
6	2.590680	2.853008	0.567946
1	3.018492	3.178218	-0.385351
1	1.613277	3.330982	0.679220
1	3.240660	3.211139	1.373600

Single point calculation:

SCF Done: E(RM062X) = -1626.75802432 A.U. after 12 cycles

TMS-TS2



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000004	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000428	0.001800	YES
RMS Displacement	0.000077	0.001200	YES

Predicted change in Energy=-6.344931D-10

Optimization completed.

SCF Done: E(RM062X) = -1626.23397349 A.U. after 6 cycles

Zero-point correction= 0.344770 (Hartree/Particle)
Thermal correction to Energy= 0.370973
Thermal correction to Enthalpy= 0.371917
Thermal correction to Gibbs Free Energy= 0.288421
Sum of electronic and zero-point Energies= -1625.889203
Sum of electronic and thermal Energies= -1625.863001
Sum of electronic and thermal Enthalpies= -1625.862057
Sum of electronic and thermal Free Energies= -1625.945553

Eigenvalues --- -0.04690 0.00094 0.00110 0.00126 0.00131

Item	Value	Threshold	Converged?
Maximum Force	0.000004	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000612	0.001800	YES
RMS Displacement	0.000103	0.001200	YES

Predicted change in Energy=-8.378118D-10
Optimization completed.

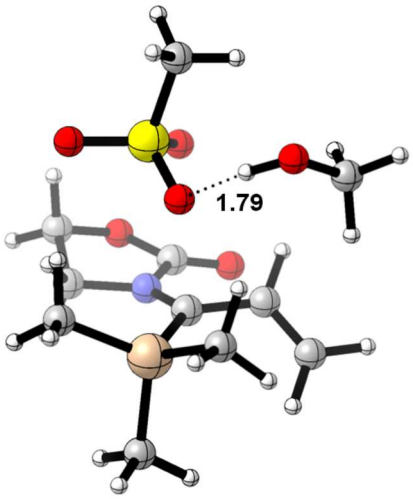
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.047992	1.493630	-1.628687
7	-1.110893	0.943194	-1.019587
6	-1.921218	2.011941	-0.430258
6	-1.016979	3.239906	-0.609004
8	0.014767	2.818881	-1.512828
8	0.924119	0.874870	-2.163335
6	-1.219459	-0.361474	-0.722481
6	-0.213206	-1.279317	-0.967610
6	0.096535	-2.373096	-1.648623
1	-2.102678	1.810739	0.625789
1	-2.867346	2.104726	-0.966745
1	-0.539870	3.528386	0.326970
1	-1.531135	4.086515	-1.060362
1	-0.484858	-2.695936	-2.509978

1	0.984520	-2.944732	-1.389558
6	3.072016	1.255844	0.526165
1	3.959574	0.649036	0.709669
1	3.234363	2.279902	0.865313
1	2.797159	1.237009	-0.530687
16	1.720070	0.580506	1.461095
8	2.097328	0.537845	2.868344
8	0.522940	1.366658	1.117682
8	1.569054	-0.854608	0.906681
1	0.655117	-0.973685	0.025094
6	3.488352	-1.702694	-1.500084
1	3.772685	-2.229998	-2.414214
1	4.341652	-1.085613	-1.184396
1	2.641923	-1.041914	-1.730775
8	3.154871	-2.678748	-0.532970
1	2.772723	-2.197725	0.220507
14	-2.603742	-1.033577	0.473567
6	-1.911084	-0.744293	2.190789
1	-2.609723	-1.117856	2.946720
1	-0.962792	-1.281249	2.301315
1	-1.711676	0.312303	2.390956
6	-4.230980	-0.144983	0.156367
1	-5.037877	-0.759706	0.569891
1	-4.288017	0.836924	0.632547
1	-4.428075	-0.025613	-0.914000
6	-2.794812	-2.852770	0.086220
1	-3.027877	-3.012043	-0.971570
1	-1.887682	-3.413189	0.323163
1	-3.620155	-3.261999	0.678656

Single point calculation:

SCF Done: E(RM062X) = -1626.72700448 A.U. after 13 cycles

TMS-I2



-- Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000003	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000616	0.001800	YES
RMS Displacement	0.000102	0.001200	YES

Predicted change in Energy=-8.847260D-10

Optimization completed.

SCF Done: E(RM062X) = -1626.27403290 A.U. after 8 cycles

Zero-point correction= 0.351481 (Hartree/Particle)

Thermal correction to Energy= 0.377627

Thermal correction to Enthalpy= 0.378571

Thermal correction to Gibbs Free Energy= 0.295915

Sum of electronic and zero-point Energies= -1625.922552

Sum of electronic and thermal Energies= -1625.896406

Sum of electronic and thermal Enthalpies= -1625.895462

Sum of electronic and thermal Free Energies= -1625.978117

Eigenvalues --- 0.00035 0.00078 0.00085 0.00111 0.00140

Item	Value	Threshold	Converged?
Maximum Force	0.000004	0.000450	YES
RMS Force	0.000001	0.000300	YES

Maximum Displacement 0.000607 0.001800 YES

RMS Displacement 0.000108 0.001200 YES

Predicted change in Energy=-1.983841D-09

Optimization completed.

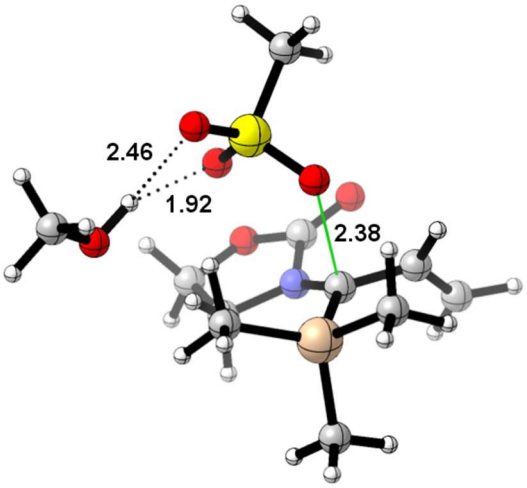
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.281978	0.166312	-1.427761
7	-1.546614	-0.545324	-0.376690
6	-2.326203	-0.458982	0.867947
6	-3.242077	0.726884	0.567479
8	-3.313690	0.769553	-0.867954
8	-2.038904	0.115092	-2.592291
6	-0.368386	-1.088702	-0.530291
6	0.324203	-0.912103	-1.812144
6	0.944420	-1.922713	-2.424688
1	-1.672371	-0.236756	1.707271
1	-2.873250	-1.393912	1.016281
1	-2.799111	1.659704	0.916615
1	-4.254365	0.595046	0.942995
1	0.954774	-2.932178	-2.024373
1	1.430661	-1.771641	-3.382380
6	1.275890	3.342195	0.743657
1	1.881081	3.255415	1.646994
1	0.672672	4.250145	0.772949
1	1.916977	3.330471	-0.138927
16	0.173654	1.944035	0.669554
8	-0.602863	1.933359	1.926389
8	-0.657915	2.110203	-0.544769
8	1.068543	0.741113	0.561504
1	0.292848	0.083574	-2.243477
6	3.351147	1.057215	-1.620008
1	4.231996	1.366085	-2.188703
1	2.500343	1.677601	-1.938838
1	3.122195	0.013039	-1.875658
8	3.643023	1.216697	-0.248937
1	2.803337	1.043533	0.219816

14	0.529195	-2.144803	0.859430
6	0.169126	-1.555358	2.601270
1	-0.808576	-1.882683	2.966131
1	0.927918	-2.008681	3.249721
1	0.253584	-0.468968	2.690521
6	-0.201940	-3.865580	0.621343
1	0.253359	-4.541354	1.354187
1	-1.282936	-3.871193	0.795181
1	-0.015538	-4.280534	-0.373382
6	2.366069	-2.128652	0.504450
1	2.633020	-2.736483	-0.363518
1	2.740992	-1.113408	0.347994
1	2.882315	-2.548113	1.375478

Single point calculation:

SCF Done: E(RM062X) = -1626.76331892 A.U. after 13 cycles

α-I4



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000004	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.000961	0.001800	YES
RMS Displacement	0.000117	0.001200	YES

Predicted change in Energy=-5.676912D-10

Optimization completed.

SCF Done: E(RM062X) = -1626.27281896 A.U. after 6 cycles

Zero-point correction= 0.350693 (Hartree/Particle)

Thermal correction to Energy= 0.377338

Thermal correction to Enthalpy= 0.378282

Thermal correction to Gibbs Free Energy= 0.294082

Sum of electronic and zero-point Energies= -1625.922125

Sum of electronic and thermal Energies= -1625.895481

Sum of electronic and thermal Enthalpies= -1625.894537

Sum of electronic and thermal Free Energies= -1625.978737

Eigenvalues --- 0.00014 0.00066 0.00105 0.00109 0.00126

Item	Value	Threshold	Converged?
Maximum Force	0.000004	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.001292	0.001800	YES
RMS Displacement	0.000156	0.001200	YES

Predicted change in Energy=-8.235772D-10

Optimization completed.

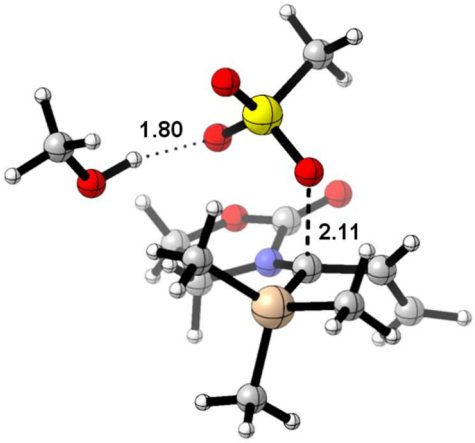
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.428557	2.311860	-0.717453
7	0.828568	0.911655	-0.874437
6	0.111391	0.324515	-2.012983
6	-0.742106	1.492096	-2.520692
8	-0.345063	2.630051	-1.740066
8	0.752591	3.036760	0.168809
6	1.492023	0.223097	0.014993
6	2.384169	0.881844	0.980252
6	3.404422	1.635973	0.570497
1	-0.529692	-0.492089	-1.683188
1	0.839545	-0.017933	-2.751028
1	-1.801360	1.313063	-2.342358
1	-0.559934	1.733791	-3.566715
1	3.531165	1.910455	-0.473146
1	4.148446	1.994691	1.273181
6	-1.965868	1.344142	2.746932
1	-1.852359	0.841777	3.707994
1	-2.999340	1.659051	2.599150
1	-1.292092	2.199159	2.677029
16	-1.539985	0.197061	1.453448

8	-2.467702	-0.942638	1.536868
8	-1.691988	0.952546	0.176242
8	-0.118562	-0.181245	1.716794
1	2.273522	0.565175	2.012129
6	-3.436136	-2.104786	-1.291768
1	-2.966182	-2.691774	-0.494342
1	-3.528714	-2.729763	-2.183770
1	-4.443147	-1.820935	-0.961223
8	-2.661394	-0.976532	-1.646055
1	-2.567937	-0.407743	-0.858592
14	1.680351	-1.717674	-0.046934
6	0.098179	-2.632906	-0.451339
1	-0.167792	-2.609500	-1.511351
1	0.255383	-3.681239	-0.170541
1	-0.743998	-2.252745	0.135330
6	2.995384	-1.951512	-1.373334
1	3.286199	-3.007075	-1.408322
1	2.645215	-1.673159	-2.372042
1	3.892335	-1.366236	-1.145857
6	2.348510	-2.211480	1.627784
1	3.317789	-1.749860	1.837220
1	1.641609	-1.934493	2.414455
1	2.482016	-3.298319	1.650879

Single point calculation:

SCF Done: E(RM062X) = -1626.76183677 A.U. after 13 cycles

TS7



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.001500	0.001800	YES
RMS Displacement	0.000212	0.001200	YES

Predicted change in Energy=-2.618973D-09

Optimization completed.

SCF Done: E(RM062X) = -1626.27234344 A.U. after 5 cycles

Zero-point correction= 0.350570 (Hartree/Particle)

Thermal correction to Energy= 0.376251

Thermal correction to Enthalpy= 0.377195

Thermal correction to Gibbs Free Energy= 0.295994

Sum of electronic and zero-point Energies= -1625.921774

Sum of electronic and thermal Energies= -1625.896093

Sum of electronic and thermal Enthalpies= -1625.895149

Sum of electronic and thermal Free Energies= -1625.976349

Eigenvalues --- -0.00591 0.00051 0.00090 0.00098 0.00142

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.001322	0.001800	YES

RMS Displacement 0.000219 0.001200 YES

Predicted change in Energy=-5.818424D-09

Optimization completed.

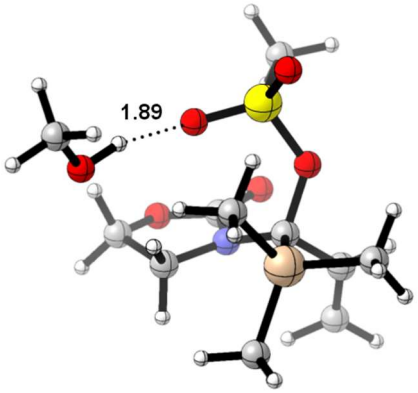
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.310080	-2.256422	0.755248
7	0.775193	-0.897874	0.915982
6	0.143778	-0.296034	2.095325
6	-0.793954	-1.408172	2.580073
8	-0.456302	-2.560826	1.794040
8	0.558899	-2.985388	-0.156723
6	1.398171	-0.223536	-0.039391
6	2.369523	-0.924954	-0.898908
6	3.325326	-1.687511	-0.367562
1	-0.420721	0.597356	1.830591
1	0.919368	-0.059397	2.826002
1	-1.839292	-1.164633	2.392678
1	-0.642771	-1.666294	3.627033
1	3.342129	-1.930199	0.691476
1	4.124819	-2.086404	-0.982195
6	-1.683485	-1.652757	-2.565004
1	-1.432552	-1.350298	-3.581965
1	-2.731271	-1.947824	-2.499491
1	-1.032668	-2.460195	-2.226437
16	-1.431657	-0.262159	-1.485386
8	-2.292113	0.835822	-1.931123
8	-1.743070	-0.753795	-0.114846
8	0.036817	0.062902	-1.626623
1	2.370176	-0.646367	-1.946658
6	-3.460998	2.183142	1.084162
1	-3.044477	2.622594	0.169530
1	-3.582202	2.971146	1.831511
1	-4.451104	1.771463	0.850503
8	-2.601434	1.200976	1.631945
1	-2.438895	0.533151	0.935173
14	1.625077	1.712417	0.014344

6	0.018737	2.668445	0.065595
1	-0.677673	2.366934	0.853375
1	0.264550	3.726278	0.218047
1	-0.497846	2.563751	-0.892763
6	2.686554	2.009774	1.540458
1	3.114281	3.016833	1.484655
1	2.114477	1.948019	2.470718
1	3.519011	1.300199	1.596274
6	2.585685	2.135637	-1.534844
1	3.569835	1.658674	-1.556219
1	2.028113	1.837786	-2.427668
1	2.734918	3.220062	-1.574965

Single point calculation:

SCF Done: E(RM062X) = -1626.76011453 A.U. after 13 cycles

α-I6



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000024	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.001020	0.001800	YES
RMS Displacement	0.000173	0.001200	YES

Predicted change in Energy=-3.093664D-09

Optimization completed.

SCF Done: E(RM062X) = -1626.28204012 A.U. after 6 cycles

Zero-point correction= 0.351502 (Hartree/Particle)

Thermal correction to Energy= 0.377465

Thermal correction to Enthalpy= 0.378410

Thermal correction to Gibbs Free Energy= 0.296210

Sum of electronic and zero-point Energies= -1625.930538

Sum of electronic and thermal Energies= -1625.904575

Sum of electronic and thermal Enthalpies= -1625.903630

Sum of electronic and thermal Free Energies= -1625.985830

Eigenvalues --- 0.00060 0.00096 0.00148 0.00164 0.00193

Item	Value	Threshold	Converged?
Maximum Force	0.000024	0.000450	YES
RMS Force	0.000002	0.000300	YES

Maximum Displacement	0.001118	0.001800	YES
RMS Displacement	0.000196	0.001200	YES

Predicted change in Energy=-3.247236D-09

Optimization completed.

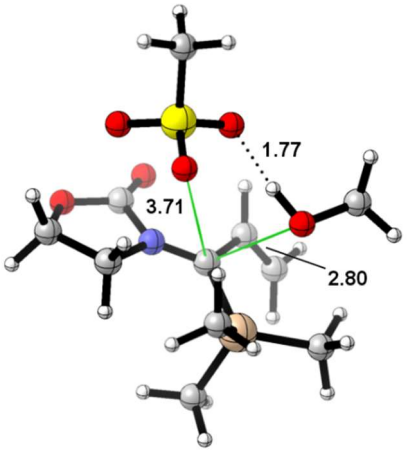
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.409801	-2.138977	-0.951846
7	-0.576925	-0.771889	-1.009328
6	0.254541	-0.185303	-2.054796
6	1.139808	-1.376970	-2.439795
8	0.472163	-2.525662	-1.895509
8	-0.928699	-2.907221	-0.176978
6	-1.247915	-0.070672	0.034875
6	-2.705583	-0.446522	0.129970
6	-3.438677	-0.806953	-0.918827
1	0.863558	0.641801	-1.688213
1	-0.367068	0.154283	-2.889242
1	2.130319	-1.302719	-1.986167
1	1.230911	-1.514173	-3.516332
1	-2.997765	-0.928679	-1.904787
1	-4.500082	-1.004591	-0.817462
6	0.775383	-2.240936	2.486781
1	0.091897	-2.250521	3.335861
1	1.794338	-2.462549	2.807113
1	0.438310	-2.919340	1.702473
16	0.788611	-0.600064	1.818815
8	1.061194	0.353737	2.878391
8	1.637935	-0.573178	0.627568
8	-0.742569	-0.463505	1.398427
1	-3.151156	-0.324209	1.113779
6	4.150688	1.812248	-0.796107
1	3.756455	2.572858	-0.109679
1	4.547087	2.317245	-1.679266
1	4.973581	1.283891	-0.299831
8	3.140420	0.923301	-1.235427
1	2.777317	0.469533	-0.455573

14	-1.165571	1.884259	-0.041669
6	0.550028	2.546773	0.336485
1	1.326491	2.196741	-0.349440
1	0.499050	3.639723	0.259677
1	0.855156	2.300101	1.357874
6	-1.764246	2.434163	-1.735700
1	-2.138066	3.461356	-1.664633
1	-0.965694	2.422760	-2.482491
1	-2.587167	1.806288	-2.092827
6	-2.342495	2.450989	1.304936
1	-3.385737	2.233025	1.059232
1	-2.101688	1.971589	2.259564
1	-2.245304	3.533403	1.440379

Single point calculation:

SCF Done: E(RM062X) = -1626.76798817 A.U. after 13 cycles

α-I5



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000002	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.001284	0.001800	YES
RMS Displacement	0.000174	0.001200	YES

Predicted change in Energy=-1.030248D-09

Optimization completed.

SCF Done: E(RM062X) = -1626.27235231 A.U. after 6 cycles

Zero-point correction= 0.351785 (Hartree/Particle)

Thermal correction to Energy= 0.377701

Thermal correction to Enthalpy= 0.378645

Thermal correction to Gibbs Free Energy= 0.297329

Sum of electronic and zero-point Energies= -1625.920567

Sum of electronic and thermal Energies= -1625.894652

Sum of electronic and thermal Enthalpies= -1625.893707

Sum of electronic and thermal Free Energies= -1625.975023

Eigenvalues --- 0.00029 0.00079 0.00099 0.00135 0.00138

Item	Value	Threshold	Converged?
Maximum Force	0.000002	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.001115	0.001800	YES

RMS Displacement 0.000158 0.001200 YES

Predicted change in Energy=-1.003947D-09

Optimization completed.

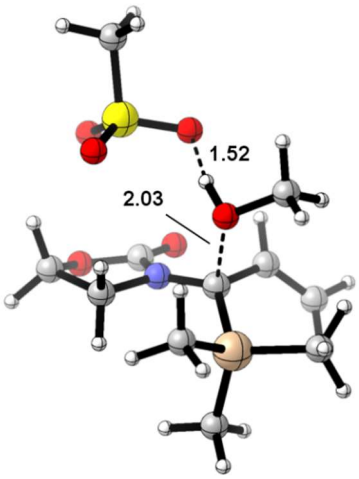
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.996237	-1.887538	1.120432
7	0.056554	-1.273732	0.168900
6	0.373088	-1.748282	-1.187451
6	1.506256	-2.755205	-0.943120
8	1.663938	-2.826890	0.479967
8	1.037736	-1.660717	2.287545
6	-1.092545	-0.077241	1.893170
6	-2.245115	-0.182635	2.560118
1	0.704033	-0.894051	-1.780877
1	-0.508517	-2.214638	-1.628003
1	2.447964	-2.406453	-1.360621
1	1.265320	-3.758547	-1.291624
1	-3.137567	-0.619117	2.119095
1	-2.313617	0.129036	3.596835
6	3.748389	2.043551	-0.361913
1	4.292223	1.951701	0.578659
1	3.423147	3.072852	-0.516042
1	4.368642	1.711254	-1.194976
16	2.305239	1.001502	-0.283944
8	1.498450	1.498459	0.869201
8	1.583018	1.170011	-1.566288
8	2.797565	-0.379334	-0.073358
1	-0.197055	0.332958	2.348550
6	-1.279036	3.135832	0.929813
1	-2.223860	3.612830	0.657354
1	-0.507399	3.909644	1.012823
1	-1.402059	2.660597	1.913662
8	-0.955402	2.197091	-0.075634
1	-0.014028	1.958414	0.067030
6	-0.970955	-0.538157	0.507330
14	-2.378753	-0.126562	-0.802663

6	-1.614007	0.379011	-2.436621
1	-1.444640	-0.476063	-3.097369
1	-2.314384	1.056413	-2.936859
1	-0.674115	0.918534	-2.288852
6	-3.250915	-1.800482	-0.943779
1	-4.043408	-1.708201	-1.695822
1	-2.606264	-2.629760	-1.248975
1	-3.730087	-2.078526	0.000995
6	-3.624958	1.105160	-0.136586
1	-3.617290	1.994802	-0.773075
1	-4.632171	0.676615	-0.143185
1	-3.393094	1.430642	0.879541

Single point calculation:

SCF Done: E(RM062X) = -1626.76069641 A.U. after 13 cycles

TS8



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000001	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.000544	0.001800	YES
RMS Displacement	0.000121	0.001200	YES

Predicted change in Energy=-3.707589D-10

Optimization completed.

SCF Done: E(RM062X) = -1626.26373272 A.U. after 6 cycles

Zero-point correction= 0.351081 (Hartree/Particle)

Thermal correction to Energy= 0.375947

Thermal correction to Enthalpy= 0.376892

Thermal correction to Gibbs Free Energy= 0.296905

Sum of electronic and zero-point Energies= -1625.912652

Sum of electronic and thermal Energies= -1625.887785

Sum of electronic and thermal Enthalpies= -1625.886841

Sum of electronic and thermal Free Energies= -1625.966828

Eigenvalues --- -0.01032 0.00016 0.00081 0.00126 0.00144

Item	Value	Threshold	Converged?
Maximum Force	0.000001	0.000450	YES
RMS Force	0.000000	0.000300	YES

Maximum Displacement	0.000663	0.001800	YES
RMS Displacement	0.000135	0.001200	YES

Predicted change in Energy=-4.263099D-10

Optimization completed.

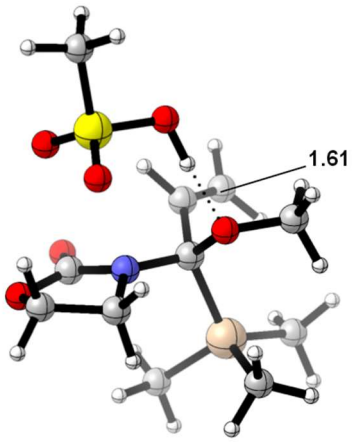
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.614132	1.769538	0.976609
7	0.223930	1.007950	0.085210
6	0.063961	1.503765	-1.286467
6	-1.152806	2.421998	-1.142530
8	-1.227363	2.705565	0.261283
8	-0.664445	1.666065	2.165459
6	1.141323	-0.295325	1.882481
6	2.242441	-0.333597	2.633785
1	-0.141959	0.668592	-1.956348
1	0.958725	2.050133	-1.597453
1	-2.071585	1.912936	-1.431720
1	-1.038100	3.369604	-1.665467
1	3.223576	-0.058096	2.257866
1	2.183944	-0.612317	3.680460
6	-4.282402	-1.660317	-0.263974
1	-4.698138	-1.762835	0.738766
1	-3.974194	-2.631467	-0.652071
1	-5.010177	-1.197073	-0.931168
16	-2.851733	-0.600876	-0.179189
8	-1.904373	-1.307605	0.758224
8	-2.283522	-0.529271	-1.541766
8	-3.300238	0.690924	0.361319
1	0.169800	-0.550974	2.294341
6	0.749530	-2.880711	0.194976
1	1.559198	-3.270369	-0.425092
1	-0.112339	-3.550729	0.133279
1	1.080558	-2.824777	1.239409
8	0.376685	-1.598956	-0.298690
1	-0.577271	-1.440552	0.024258
6	1.155959	0.113751	0.463244

14	2.774908	-0.080245	-0.614091
6	2.377267	-0.396120	-2.419287
1	2.090522	0.504155	-2.967547
1	3.279661	-0.798150	-2.893079
1	1.580900	-1.139096	-2.518173
6	3.680541	1.552321	-0.380411
1	4.621233	1.522035	-0.941317
1	3.105962	2.409536	-0.744663
1	3.924606	1.734920	0.670889
6	3.802418	-1.506599	0.062881
1	4.091659	-2.171991	-0.756720
1	4.720942	-1.123085	0.519373
1	3.285438	-2.104619	0.815522

Single point calculation:

SCF Done: E(RM062X) = -1626.75169407 A.U. after 13 cycles

α-I7



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000018	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.000923	0.001800	YES
RMS Displacement	0.000232	0.001200	YES

Predicted change in Energy=-5.061606D-09

Optimization completed.

SCF Done: E(RM062X) = -1626.28756577 A.U. after 7 cycles

Zero-point correction= 0.352359 (Hartree/Particle)

Thermal correction to Energy= 0.377141

Thermal correction to Enthalpy= 0.378085

Thermal correction to Gibbs Free Energy= 0.298946

Sum of electronic and zero-point Energies= -1625.935206

Sum of electronic and thermal Energies= -1625.910425

Sum of electronic and thermal Enthalpies= -1625.909481

Sum of electronic and thermal Free Energies= -1625.988620

Eigenvalues --- 0.00071 0.00091 0.00149 0.00222 0.00263

Item	Value	Threshold	Converged?
Maximum Force	0.000018	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.001797	0.001800	YES

RMS Displacement 0.000362 0.001200 YES

Predicted change in Energy=-8.472454D-09

Optimization completed.

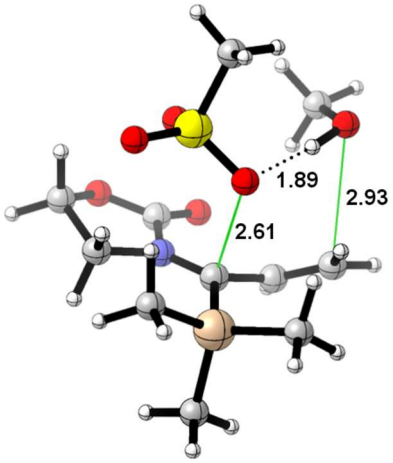
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.001822	1.738605	0.946526
7	0.155502	0.770056	-0.025111
6	-0.039667	1.361593	-1.346186
6	-0.924340	2.548630	-0.969633
8	-0.559297	2.835694	0.386832
8	0.311507	1.691492	2.111539
6	0.645645	-0.975099	1.573308
6	1.441410	-1.760583	2.293661
1	-0.540919	0.669673	-2.022772
1	0.911649	1.689013	-1.786729
1	-1.981345	2.278265	-0.998642
1	-0.736085	3.438656	-1.568954
1	2.445209	-2.029530	1.986115
1	1.098774	-2.164565	3.240965
6	-4.632279	-1.140771	0.161991
1	-4.646795	-1.574421	1.161810
1	-4.793892	-1.901270	-0.601268
1	-5.372844	-0.344314	0.079724
16	-3.045939	-0.399071	-0.104638
8	-2.140301	-1.690681	0.088342
8	-2.933572	0.052316	-1.488073
8	-2.784633	0.567913	0.951889
1	-0.355860	-0.744914	1.931615
6	0.954405	-2.618892	-0.925193
1	1.932699	-2.497674	-1.402722
1	0.308655	-3.204097	-1.580426
1	1.069244	-3.130755	0.035096
8	0.316857	-1.358178	-0.764252
1	-1.214258	-1.527843	-0.291825
6	0.943135	-0.444871	0.187225
14	2.802642	-0.048469	-0.310237

6	2.864278	-0.094472	-2.202327
1	3.112518	0.892272	-2.607540
1	3.630886	-0.796541	-2.546706
1	1.907655	-0.403057	-2.635832
6	3.129781	1.674690	0.361144
1	4.182298	1.938010	0.212082
1	2.520609	2.436556	-0.137760
1	2.909414	1.722002	1.431981
6	4.128532	-1.213100	0.351165
1	5.061314	-0.970204	-0.171779
1	4.306915	-1.074444	1.420958
1	3.914725	-2.270329	0.165614

Single point calculation:

SCF Done: E(RM062X) = -1626.77303824 A.U. after 12 cycles

γ-I5



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000023	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.001422	0.001800	YES
RMS Displacement	0.000277	0.001200	YES

Predicted change in Energy=-1.393210D-08

Optimization completed.

SCF Done: E(RM062X) = -1626.27388742 A.U. after 7 cycles

Zero-point correction= 0.352792 (Hartree/Particle)

Thermal correction to Energy= 0.378331

Thermal correction to Enthalpy= 0.379276

Thermal correction to Gibbs Free Energy= 0.299109

Sum of electronic and zero-point Energies= -1625.921095

Sum of electronic and thermal Energies= -1625.895556

Sum of electronic and thermal Enthalpies= -1625.894612

Sum of electronic and thermal Free Energies= -1625.974778

Eigenvalues --- 0.00098 0.00116 0.00136 0.00201 0.00290

Item	Value	Threshold	Converged?
Maximum Force	0.000023	0.000450	YES
RMS Force	0.000003	0.000300	YES

Maximum Displacement 0.001652 0.001800 YES

RMS Displacement 0.000316 0.001200 YES

Predicted change in Energy=-1.422010D-08

Optimization completed.

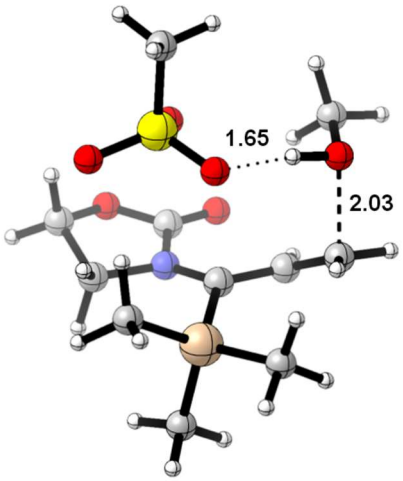
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.500483	1.949263	1.425393
7	0.533541	1.307440	0.614932
6	0.793332	2.145249	-0.566820
6	-0.355298	3.153806	-0.517334
8	-0.874265	3.058893	0.817904
8	-0.891198	1.568297	2.485562
6	1.033687	0.115017	0.827572
6	0.728651	-0.581691	2.081088
6	0.481446	-1.895819	2.122276
1	0.733950	1.544267	-1.472449
1	1.776000	2.612350	-0.462631
1	-1.152924	2.876074	-1.204870
1	-0.031252	4.181109	-0.671508
1	0.459151	-2.510479	1.231697
1	0.225816	-2.374234	3.061600
6	-2.800335	-1.291817	-1.992856
1	-2.437933	-1.992266	-2.746146
1	-3.566324	-0.639441	-2.413271
1	-3.179398	-1.831787	-1.122618
16	-1.431073	-0.285739	-1.456589
8	-0.857516	0.356858	-2.656417
8	-1.971684	0.679489	-0.470275
8	-0.473567	-1.249932	-0.812027
1	0.659552	0.016812	2.981518
6	-2.906496	-1.345292	1.806888
1	-3.570968	-0.790394	1.132920
1	-2.210872	-0.625532	2.256154
1	-3.507351	-1.799463	2.599392
8	-2.228860	-2.394046	1.138717
1	-1.578811	-1.990222	0.532555

14	2.469512	-0.611778	-0.289984
6	3.947326	0.141135	0.604306
1	4.869059	-0.187529	0.111927
1	3.932489	1.235943	0.584043
1	3.990563	-0.182124	1.649129
6	2.441944	-0.094328	-2.089019
1	2.777481	0.934096	-2.246284
1	3.147002	-0.752338	-2.610435
1	1.453647	-0.226946	-2.539052
6	2.541888	-2.477751	-0.199323
1	2.702795	-2.863899	0.809429
1	1.643036	-2.929315	-0.627688
1	3.397249	-2.783138	-0.813475

Single point calculation:

SCF Done: E(RM062X) = -1626.76262340 A.U. after 13 cycles

TS9



— Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000015	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.000588	0.001800	YES
RMS Displacement	0.000148	0.001200	YES

Predicted change in Energy=-1.870866D-09

Optimization completed.

SCF Done: E(RM062X) = -1626.26515522 A.U. after 9 cycles

Zero-point correction= 0.353297 (Hartree/Particle)

Thermal correction to Energy= 0.377634

Thermal correction to Enthalpy= 0.378578

Thermal correction to Gibbs Free Energy= 0.300660

Sum of electronic and zero-point Energies= -1625.911859

Sum of electronic and thermal Energies= -1625.887521

Sum of electronic and thermal Enthalpies= -1625.886577

Sum of electronic and thermal Free Energies= -1625.964495

Eigenvalues --- -0.01736 0.00093 0.00131 0.00187 0.00253

Item	Value	Threshold	Converged?
Maximum Force	0.000015	0.000450	YES
RMS Force	0.000002	0.000300	YES

Maximum Displacement	0.000654	0.001800	YES
RMS Displacement	0.000177	0.001200	YES

Predicted change in Energy=-2.202760D-09

Optimization completed.

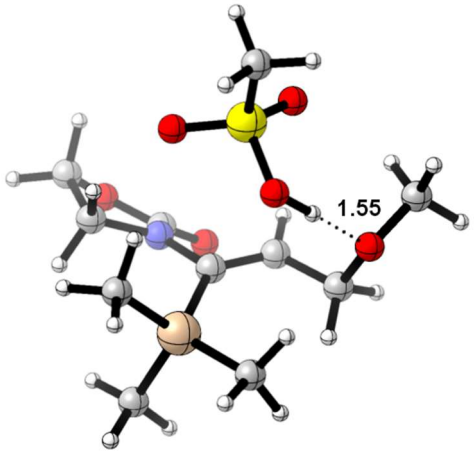
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.503228	1.674290	1.772082
7	0.485826	1.244934	0.823493
6	0.645920	2.299778	-0.188331
6	-0.631129	3.110956	0.006582
8	-1.025804	2.823432	1.355055
8	-0.793817	1.145902	2.807276
6	1.022898	0.012097	0.753767
6	0.798995	-0.913220	1.794858
6	0.824311	-2.276801	1.578752
1	0.673409	1.875562	-1.188823
1	1.546936	2.882114	0.023226
1	-1.418880	2.766596	-0.663728
1	-0.476643	4.185267	-0.074851
1	1.217885	-2.714895	0.673063
1	0.723151	-2.951730	2.421466
6	-3.181288	-0.875563	-2.066709
1	-2.890562	-1.288180	-3.033197
1	-3.931922	-0.094988	-2.195233
1	-3.562709	-1.663208	-1.415238
16	-1.741066	-0.149414	-1.303852
8	-1.251036	0.890605	-2.230272
8	-2.175264	0.368619	0.010222
8	-0.759394	-1.280555	-1.167883
1	0.407106	-0.561228	2.737753
6	-2.019871	-2.272919	1.810936
1	-2.998445	-2.311399	1.322690
1	-1.793463	-1.228995	2.053815
1	-2.044858	-2.877857	2.719791
8	-1.030833	-2.832275	0.954048
1	-1.013707	-2.288064	0.116586

14	2.412404	-0.286213	-0.594669
6	3.794864	0.774231	0.126463
1	4.686958	0.664463	-0.500189
1	3.550398	1.839435	0.168131
1	4.052254	0.443731	1.137917
6	1.992854	0.233086	-2.348880
1	2.295785	1.264512	-2.553682
1	2.555024	-0.417736	-3.027615
1	0.928139	0.125302	-2.570084
6	3.055288	-2.048582	-0.651333
1	3.371524	-2.435333	0.320785
1	2.353146	-2.748798	-1.112950
1	3.943603	-2.011452	-1.293773

Single point calculation:

SCF Done: E(RM062X) = -1626.75204680 A.U. after 14 cycles

γ-I7



-- Stationary point found.

Item	Value	Threshold	Converged?
Maximum Force	0.000003	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.011311	0.001800	NO
RMS Displacement	0.002563	0.001200	NO

Predicted change in Energy=-3.115912D-07

Optimization completed on the basis of negligible forces.

SCF Done: E(RM062X) = -1626.29664557 A.U. after 8 cycles

Zero-point correction= 0.353877 (Hartree/Particle)

Thermal correction to Energy= 0.378726

Thermal correction to Enthalpy= 0.379670

Thermal correction to Gibbs Free Energy= 0.299011

Sum of electronic and zero-point Energies= -1625.942768

Sum of electronic and thermal Energies= -1625.917920

Sum of electronic and thermal Enthalpies= -1625.916976

Sum of electronic and thermal Free Energies= -1625.997635

Eigenvalues --- 0.00089 0.00110 0.00136 0.00241 0.00255

Item	Value	Threshold	Converged?
Maximum Force	0.000003	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000177	0.001800	YES

RMS Displacement 0.000052 0.001200 YES

Predicted change in Energy=-2.235289D-10

Optimization completed.

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.478916	-1.099234	1.381813
7	-1.739903	-0.597650	0.329457
6	-2.198593	-1.179110	-0.927942
6	-2.862642	-2.450144	-0.407562
8	-3.258824	-2.113957	0.926676
8	-2.500091	-0.737825	2.532661
6	-0.851158	0.508517	0.440115
6	-0.085604	0.559563	1.545444
6	0.834743	1.681118	1.921978
1	-1.359217	-1.388728	-1.589008
1	-2.921018	-0.522535	-1.429828
1	-2.151776	-3.280324	-0.362051
1	-3.749239	-2.745149	-0.966952
1	0.557761	2.621975	1.454153
1	0.829150	1.831957	3.007168
6	3.493443	-1.831200	-1.593647
1	3.427644	-1.421262	-2.601610
1	3.466872	-2.921161	-1.620733
1	4.390598	-1.477925	-1.085842
16	2.076503	-1.286724	-0.674862
8	0.880289	-1.697180	-1.395780
8	2.220553	-1.674855	0.722257
8	2.242392	0.285507	-0.789309
1	-0.126144	-0.275765	2.239669
6	2.946956	0.700399	2.491133
1	3.918641	0.485329	2.044577
1	2.454737	-0.240769	2.748766
1	3.078974	1.321289	3.382893
8	2.195010	1.424407	1.518842
1	2.215304	0.714302	0.142640
14	-0.975813	1.803837	-0.975160

6	-2.717738	2.513423	-0.873824
1	-2.889688	3.220037	-1.692992
1	-3.482541	1.732555	-0.938878
1	-2.865555	3.046500	0.070842
6	-0.693991	1.009570	-2.662158
1	-1.588620	0.522037	-3.058492
1	-0.409107	1.799653	-3.365905
1	0.114977	0.274704	-2.626470
6	0.266647	3.215663	-0.844591
1	0.019056	3.936664	-0.060222
1	1.294840	2.871176	-0.695483
1	0.237493	3.752686	-1.799726

Single point calculation:

SCF Done: E(RM062X) = -1626.78292529 A.U. after 12 cycles

6. References

(1) Lu, T.; Lu, Z.; Ma, Z.-X.; Zhang, Y.; Hsung, R. P. Allenamides: A Powerful and Versatile Building Block in Organic Synthesis. *Chem. Rev.* **2013**, *113* (7), 4862–4904. https://doi.org/10.1021/cr400015d.

(2) Motiwala, H. F.; Armaly, A. M.; Cacioppo, J. G.; Coombs, T. C.; Koehn, K. R. K.; Norwood, V. M. I.; Aubé, J. HFIP in Organic Synthesis. *Chem. Rev.* **2022**, *122* (15), 12544–12747. https://doi.org/10.1021/acs.chemrev.1c00749.

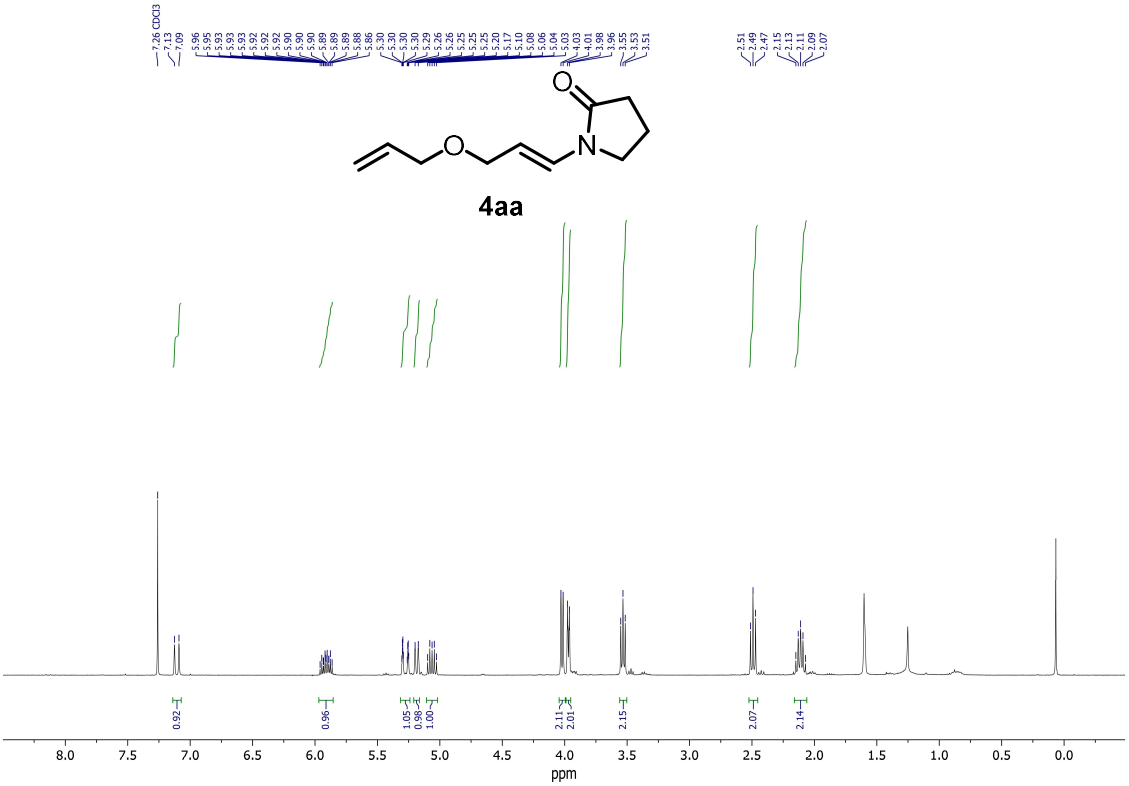
(3) Bordwell, F. G. Equilibrium Acidities in Dimethyl Sulfoxide Solution. *Acc. Chem. Res.* **1988**, *21* (12), 456–463. https://doi.org/10.1021/ar00156a004.

(4) Dyatkin, B. L.; Mochalina, E. P.; Knunyants, I. L. The Acidic Properties of Fluorine-Containing Alcohols, Hydroxylamines and Oximes. *Tetrahedron* **1965**, *21* (11), 2991–2995. https://doi.org/10.1016/S0040-4020(01)96918-2.

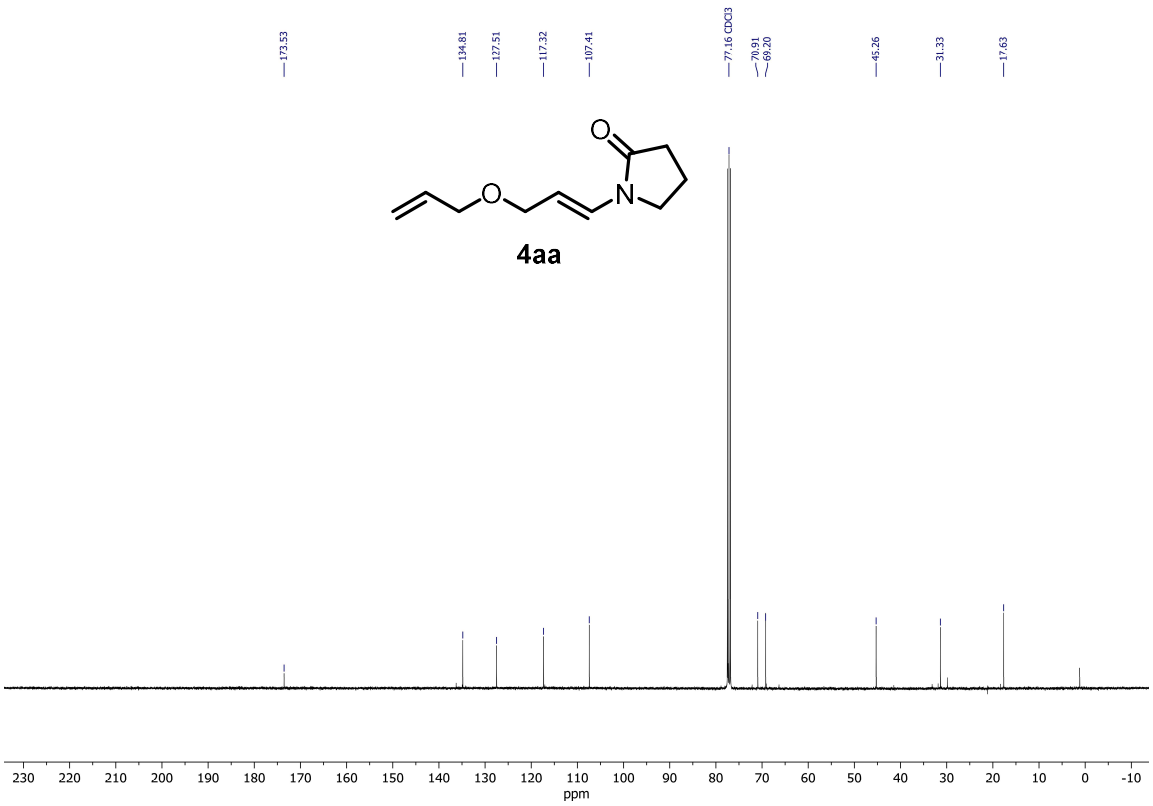
(5) Pozhydaiev, V.; Power, M.; Gandon, V.; Moran, J.; Lebœuf, D. Exploiting Hexafluoroisopropanol (HFIP) in Lewis and Brønsted Acid-Catalyzed Reactions. *Chem. Commun.* **2020**, *56* (78), 11548–11564. https://doi.org/10.1039/D0CC05194B.

7. NMR spectra

^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



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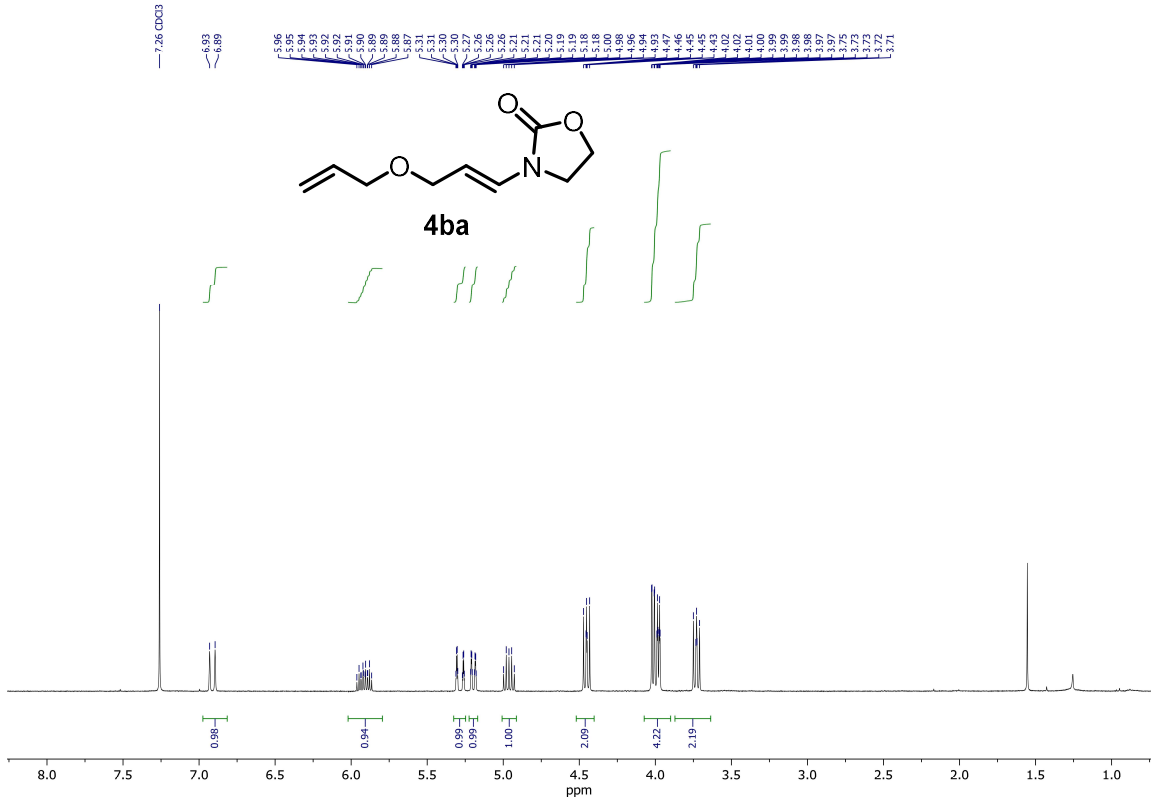
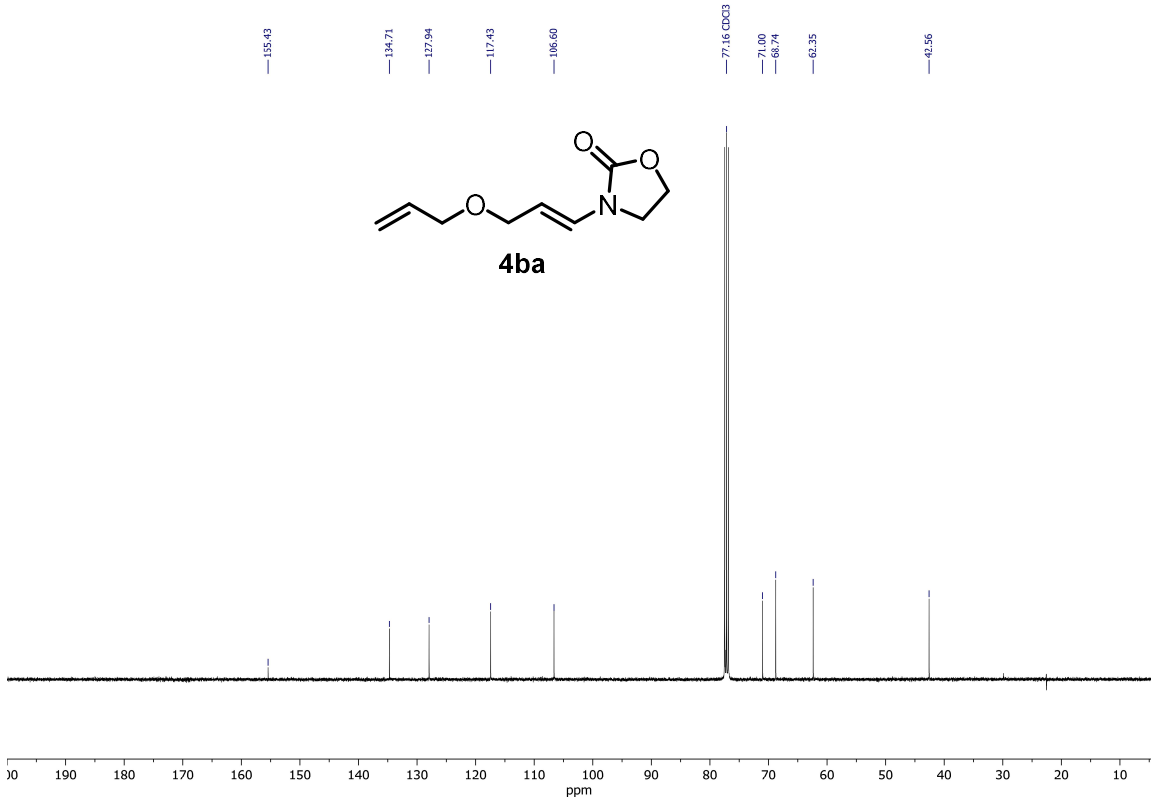
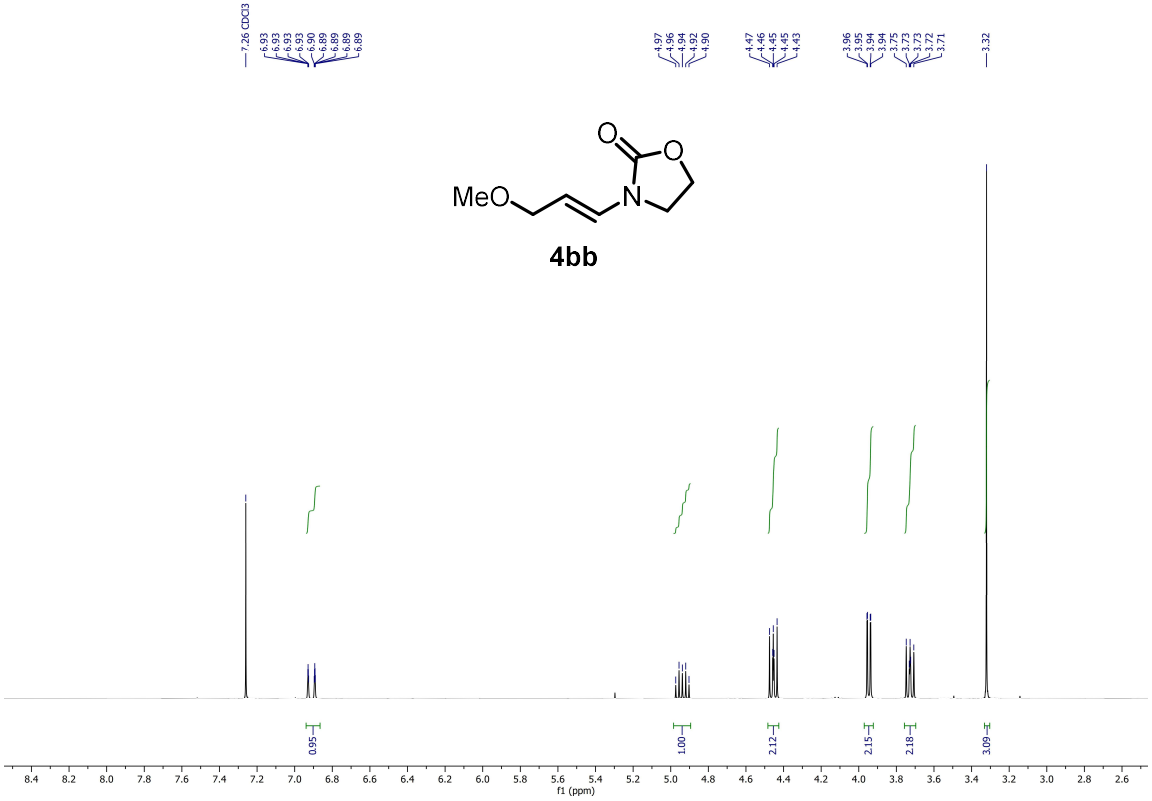


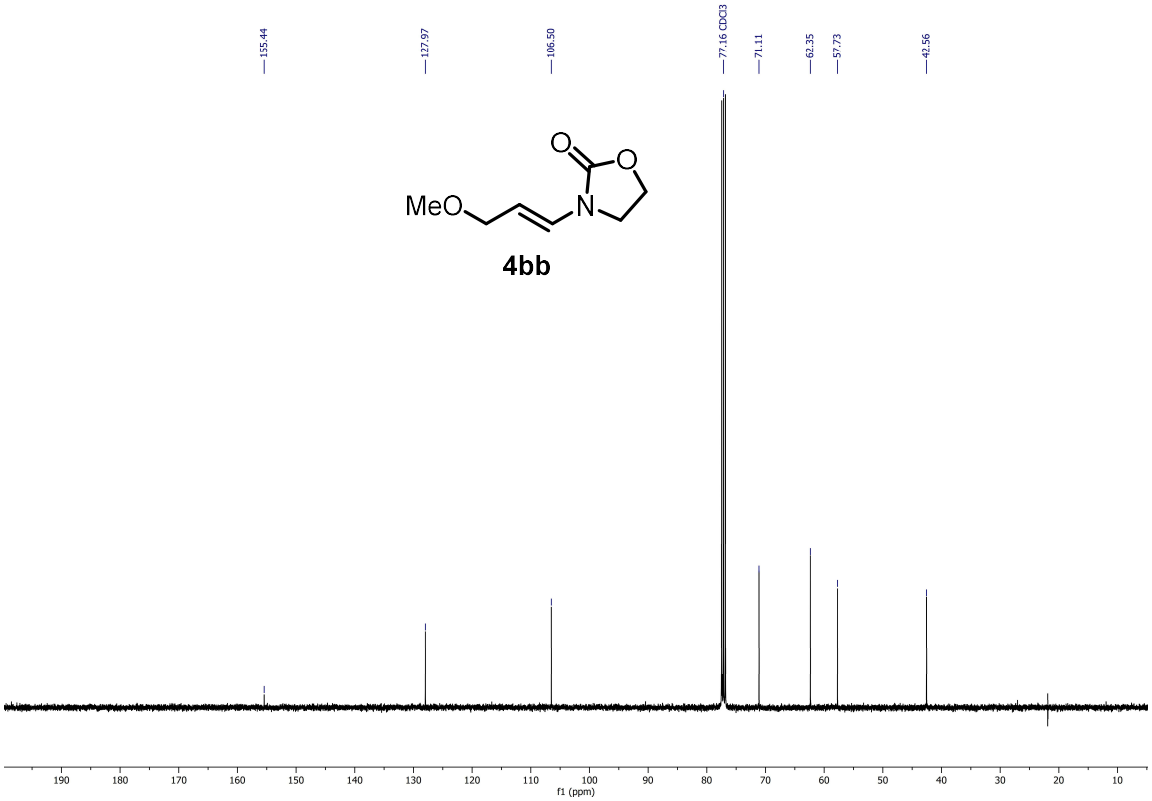
^{13}C NMR (100 MHz, $CDCl_3$)



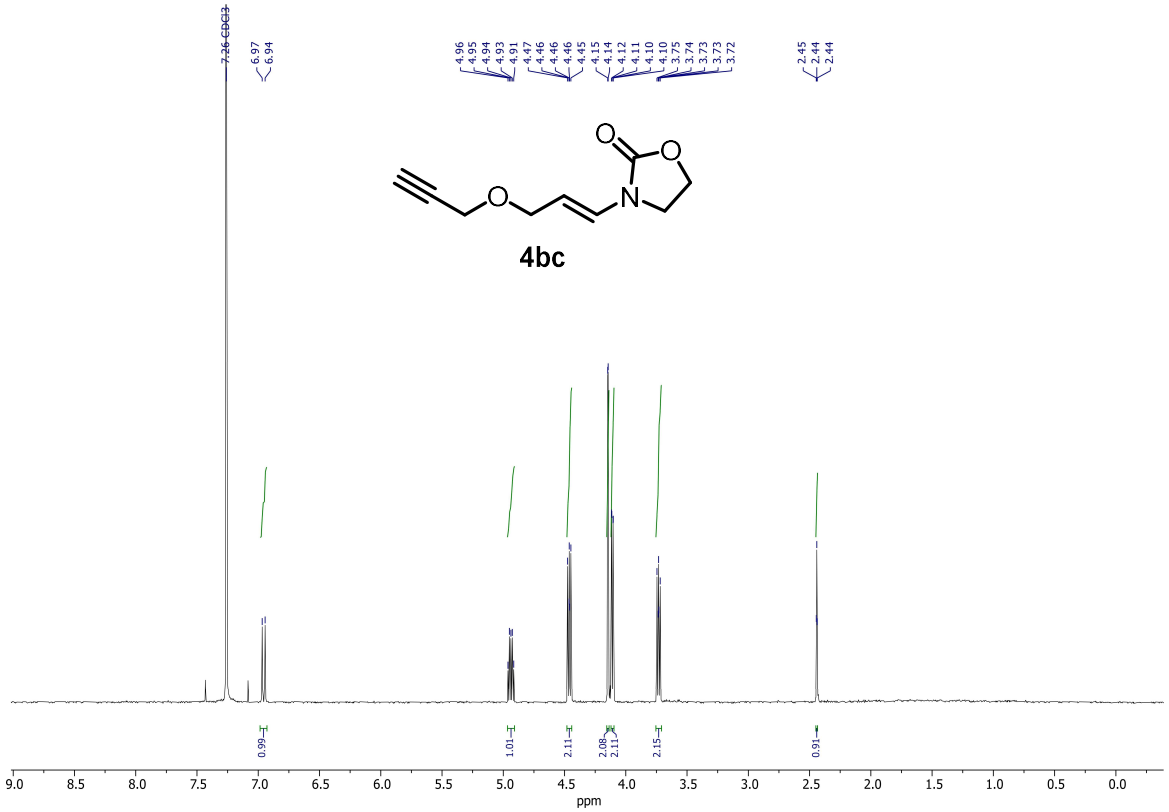
^{1}H NMR (400 MHz, $CDCl_3$)



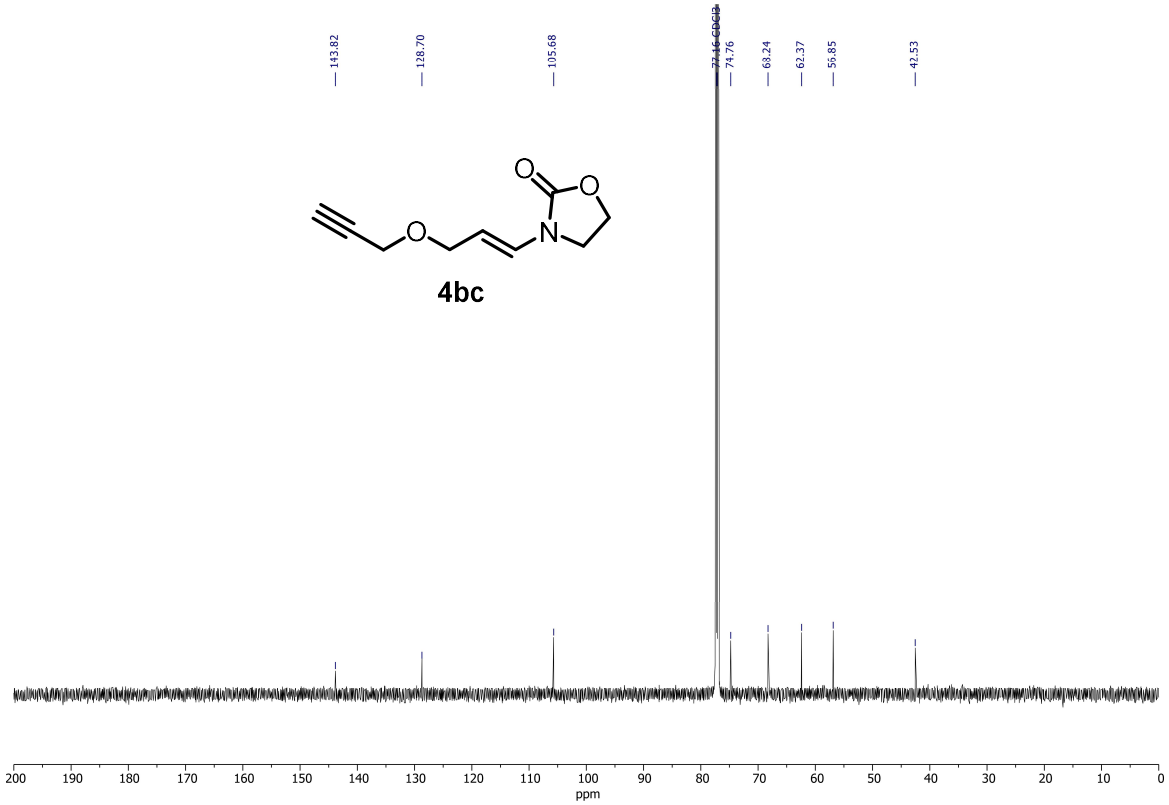
^{13}C NMR (100 MHz, $CDCl_3$)



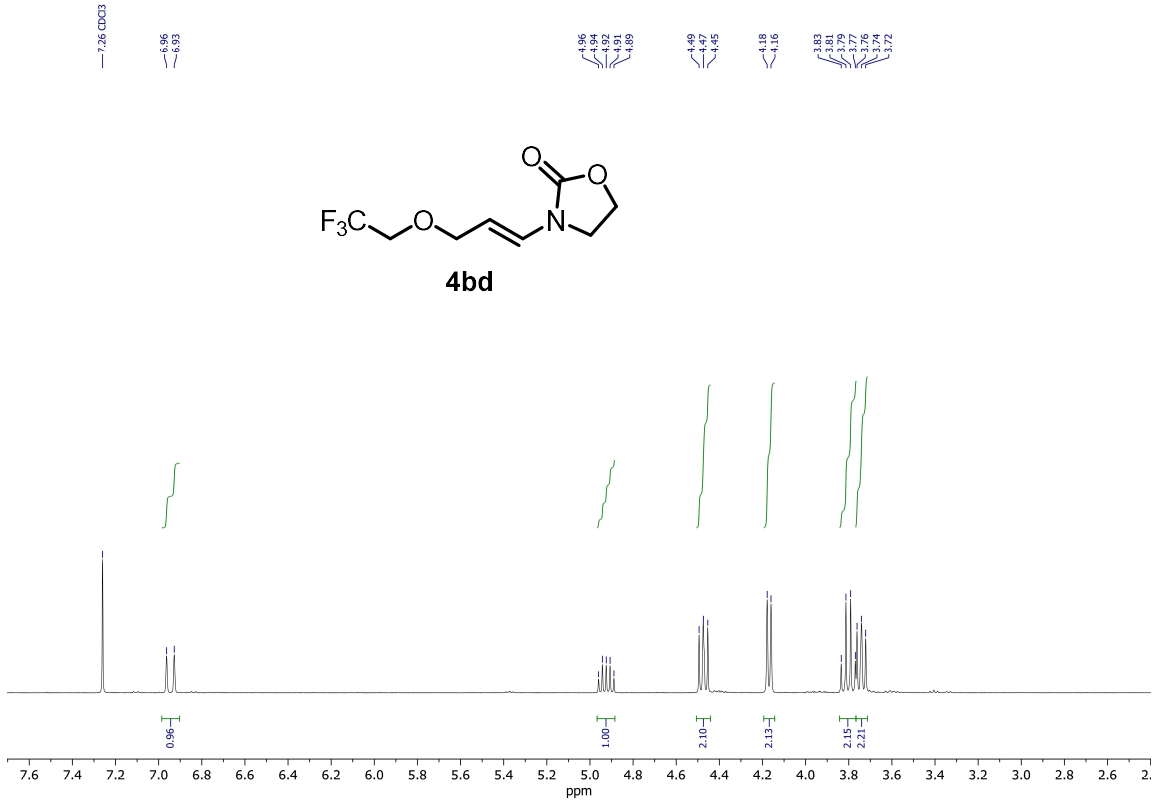
^{1}H NMR (400 MHz, $CDCl_3$)



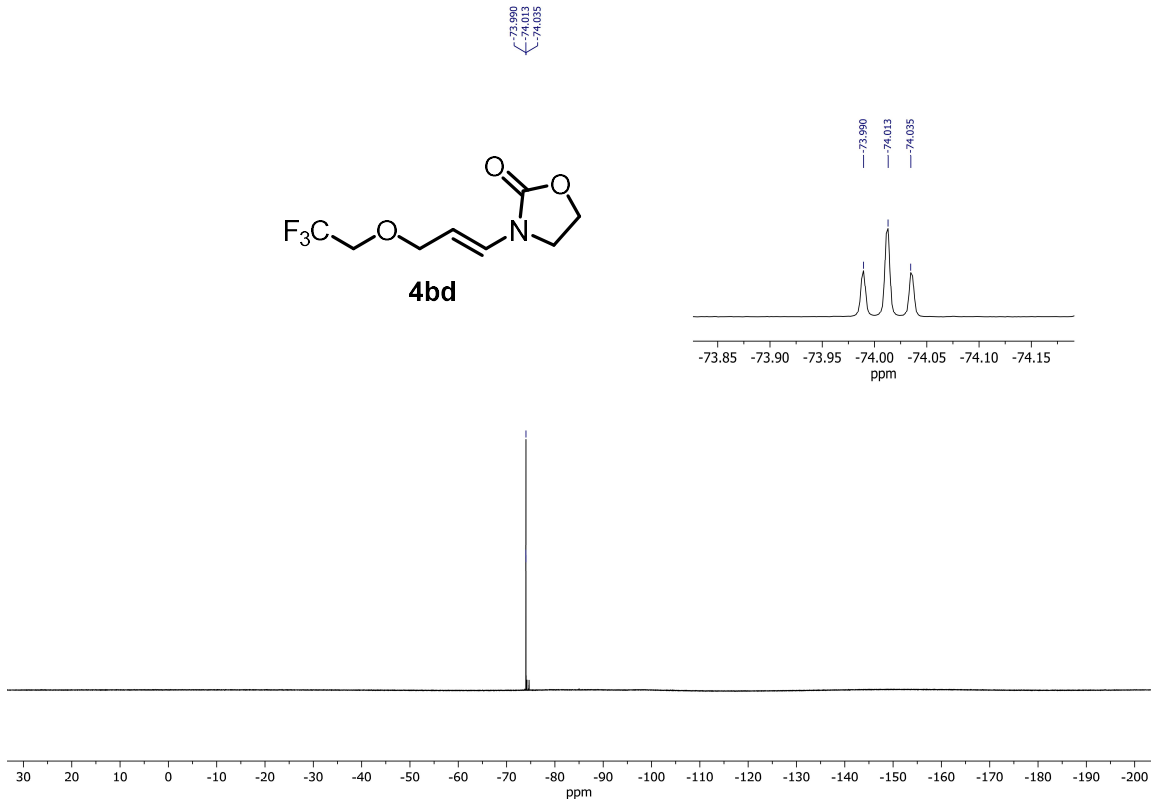
^{13}C NMR (100 MHz, $CDCl_3$)



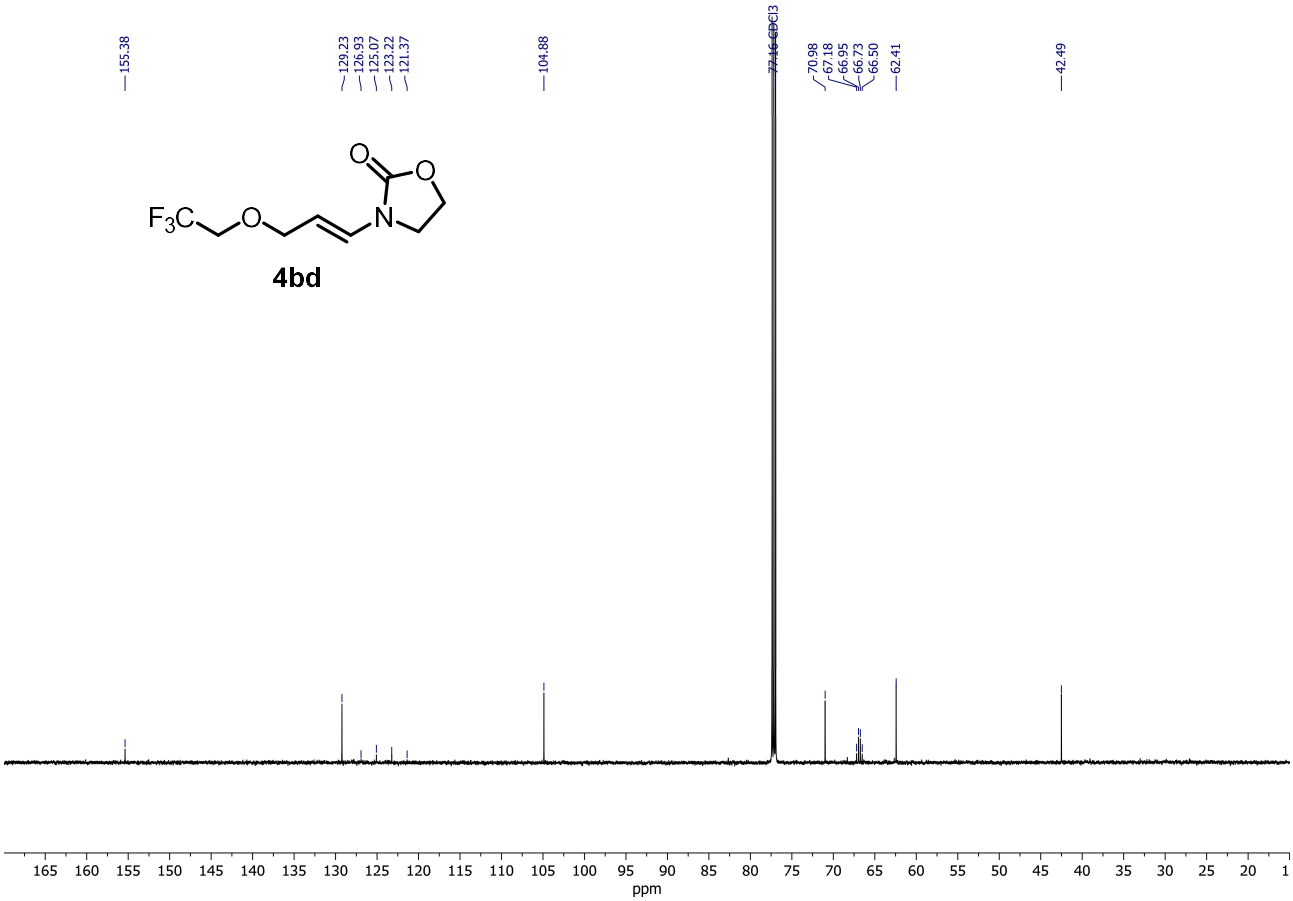
^{1}H NMR (400 MHz, $CDCl_3$)



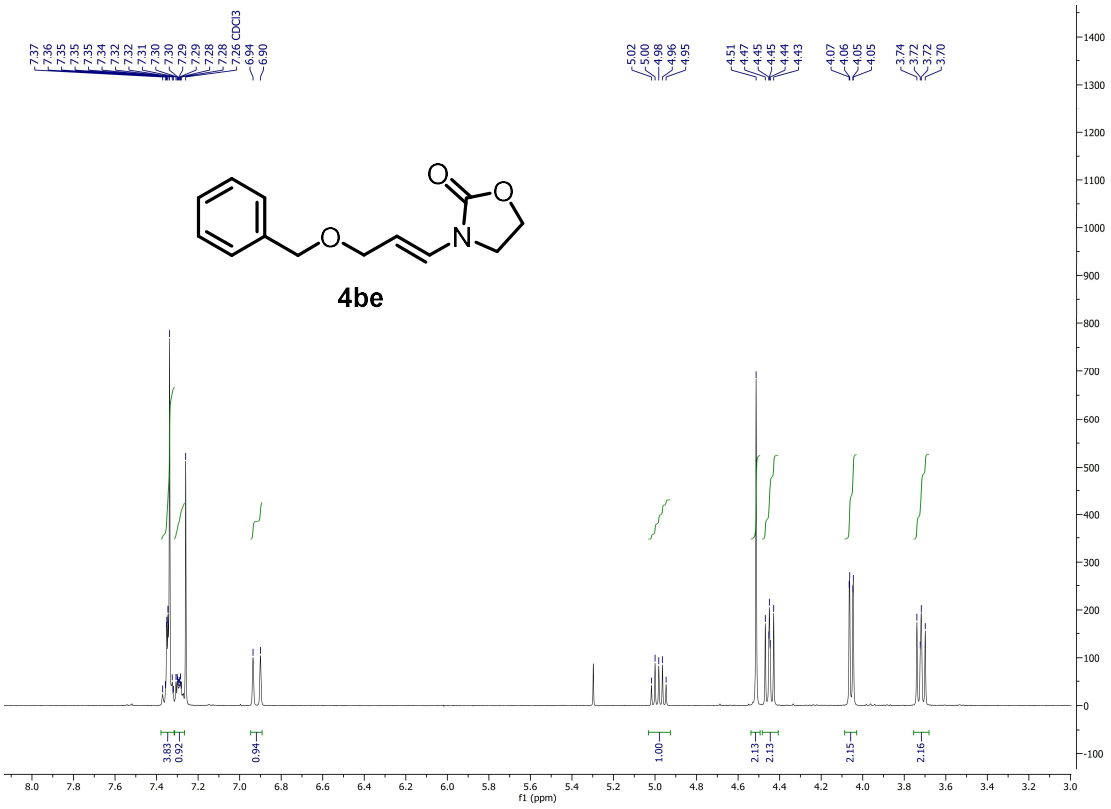
^{19}F NMR (376 MHz, $CDCl_3$)



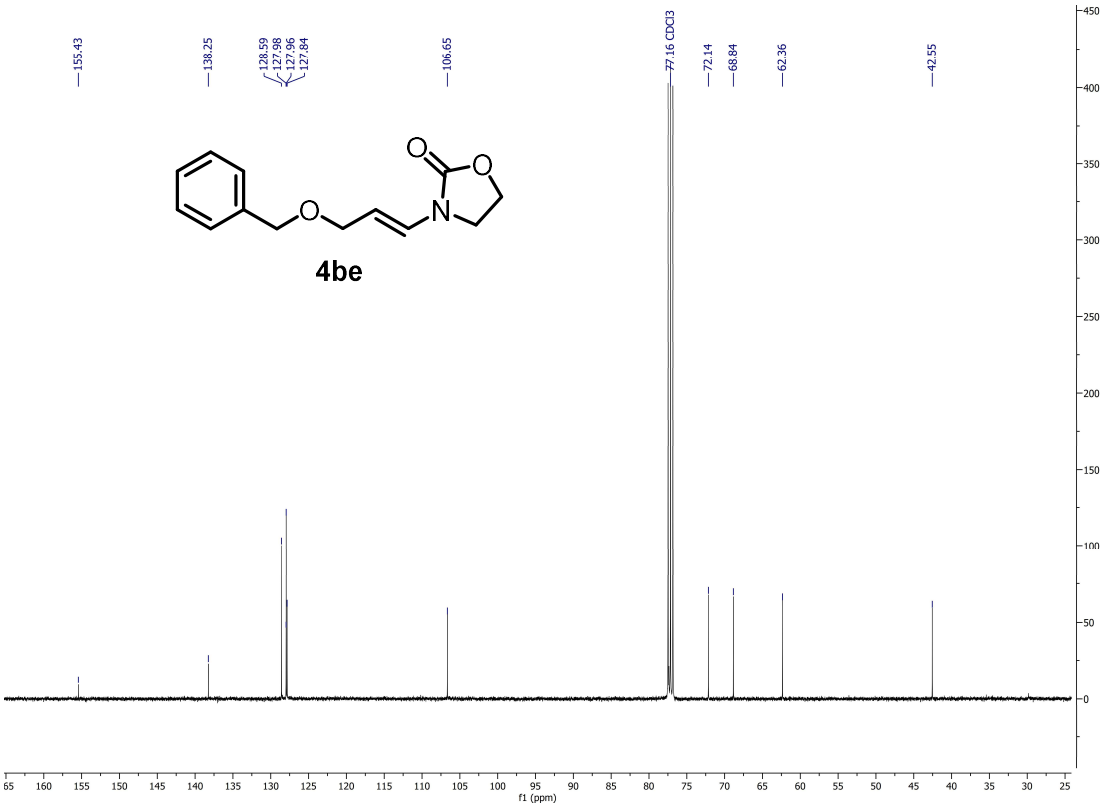
^{13}C NMR (150 MHz, $CDCl_3$)



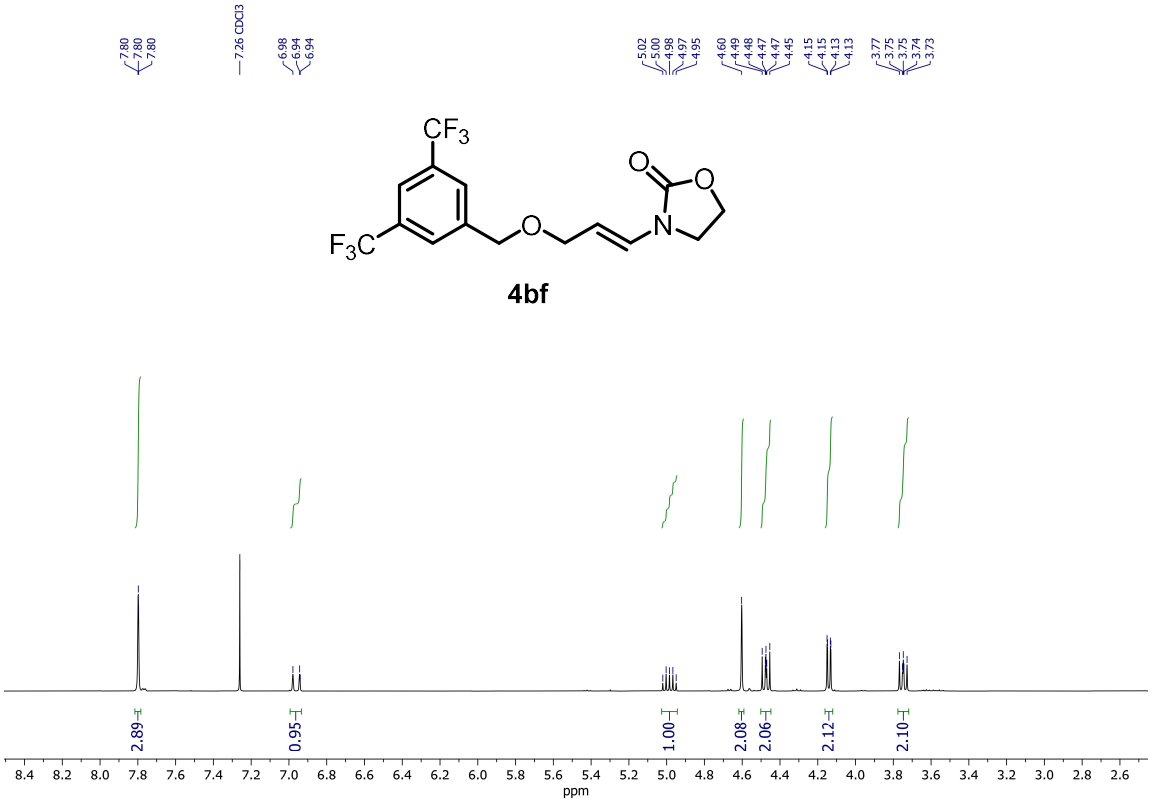
^{1}H NMR (400 MHz, $CDCl_3$)



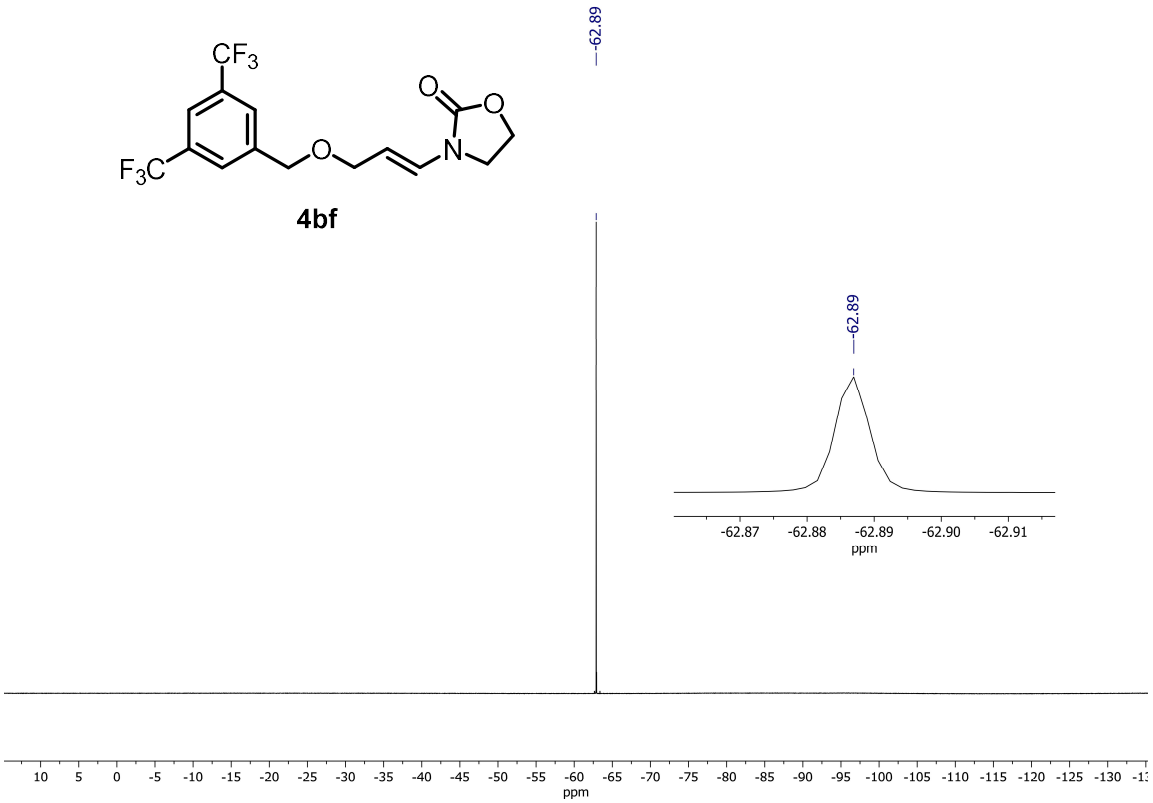
^{13}C NMR (100 MHz, $CDCl_3$)



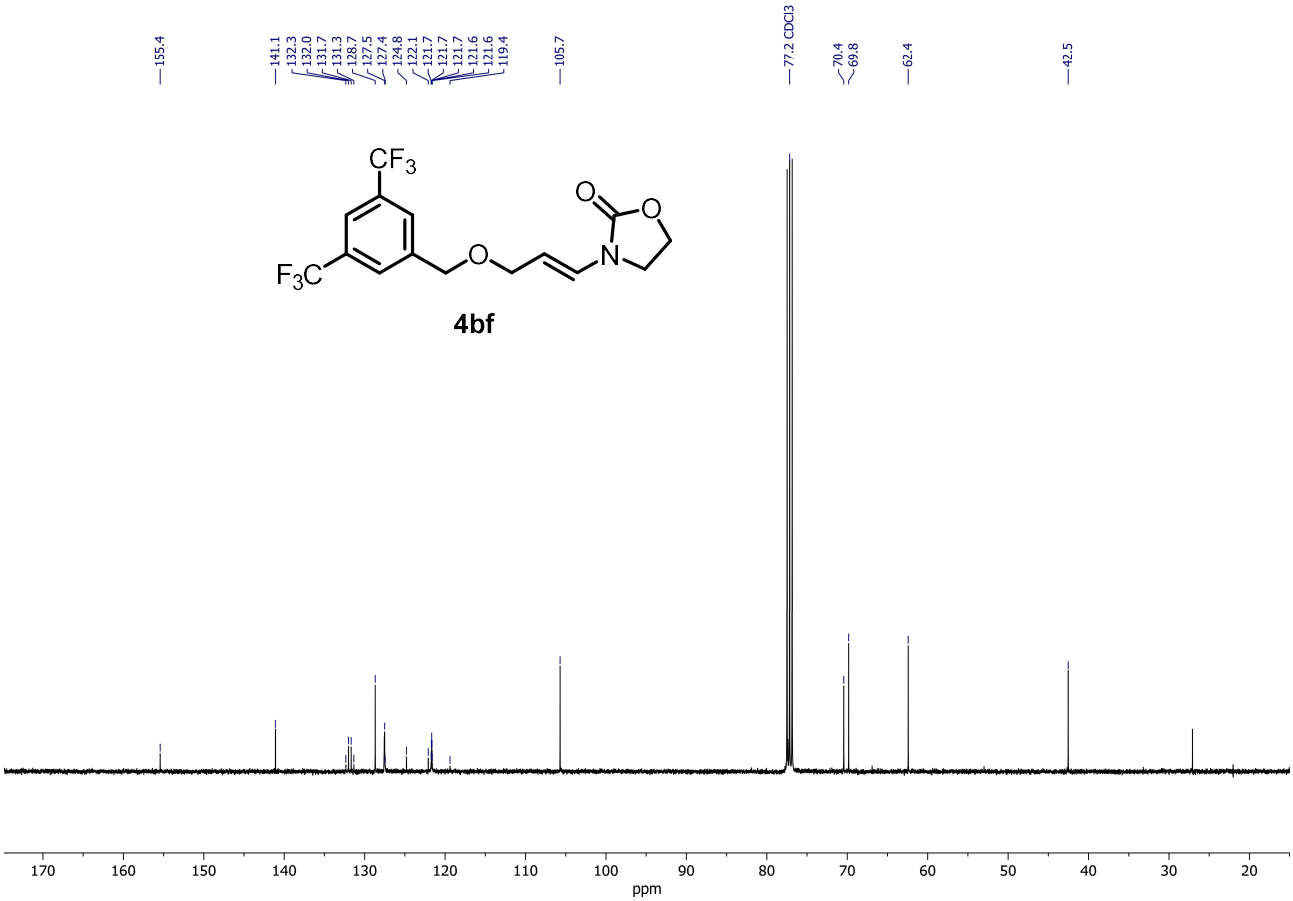
^{1}H NMR (400 MHz, $CDCl_3$)



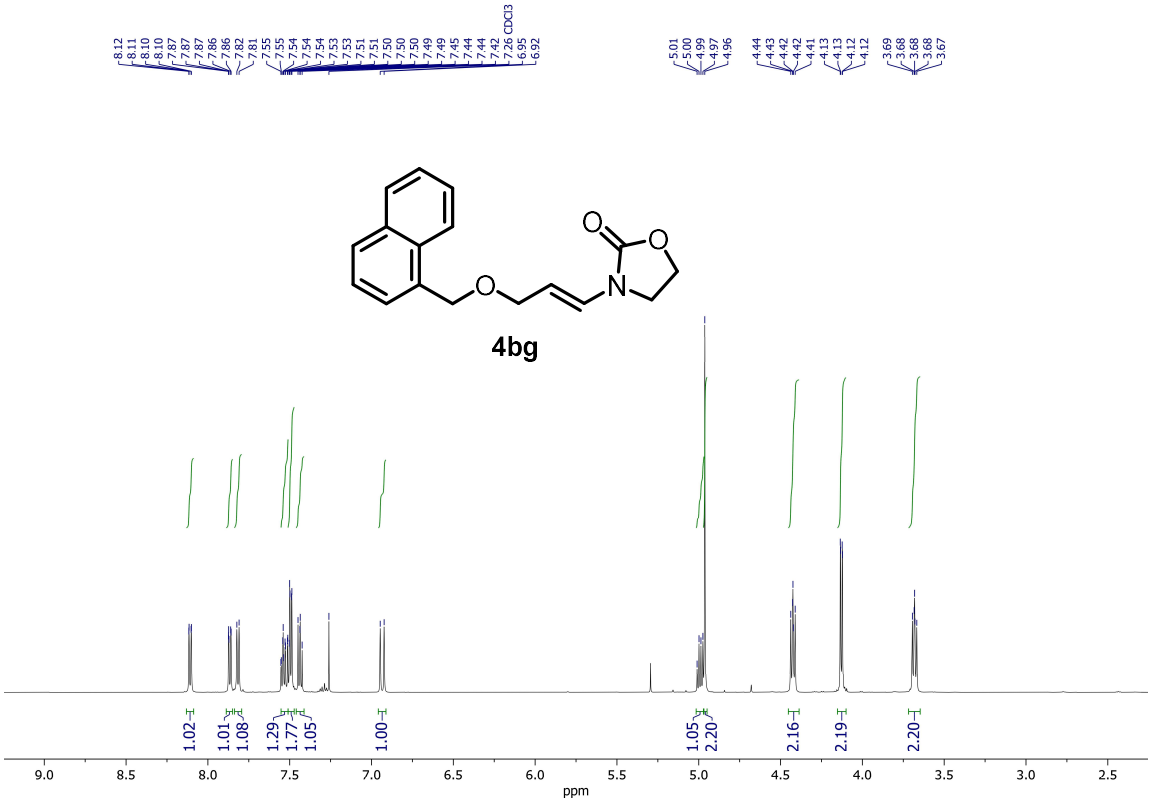
^{19}F NMR (376 MHz, $CDCl_3$)



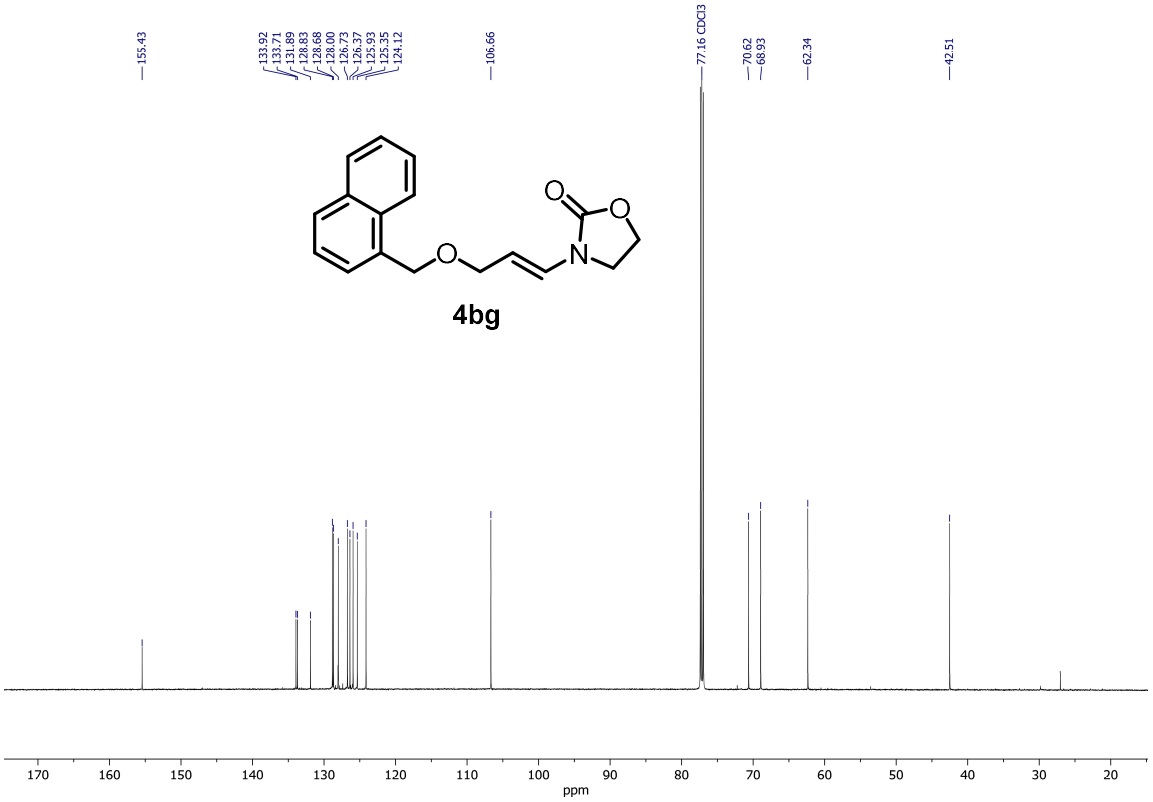
^{13}C NMR (100 MHz, $CDCl_3$)



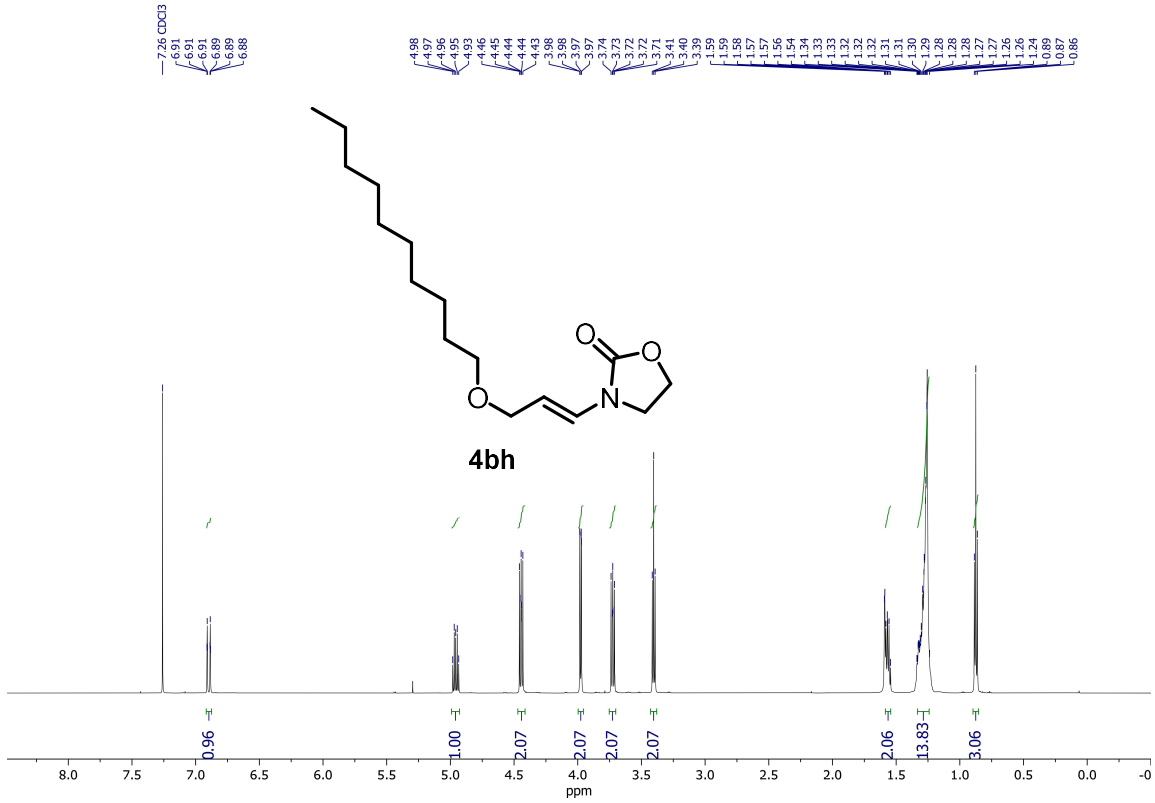
^{1}H NMR (600 MHz, $CDCl_3$)



^{13}C NMR (150 MHz, $CDCl_3$)



^{1}H NMR (600 MHz, $CDCl_3$)



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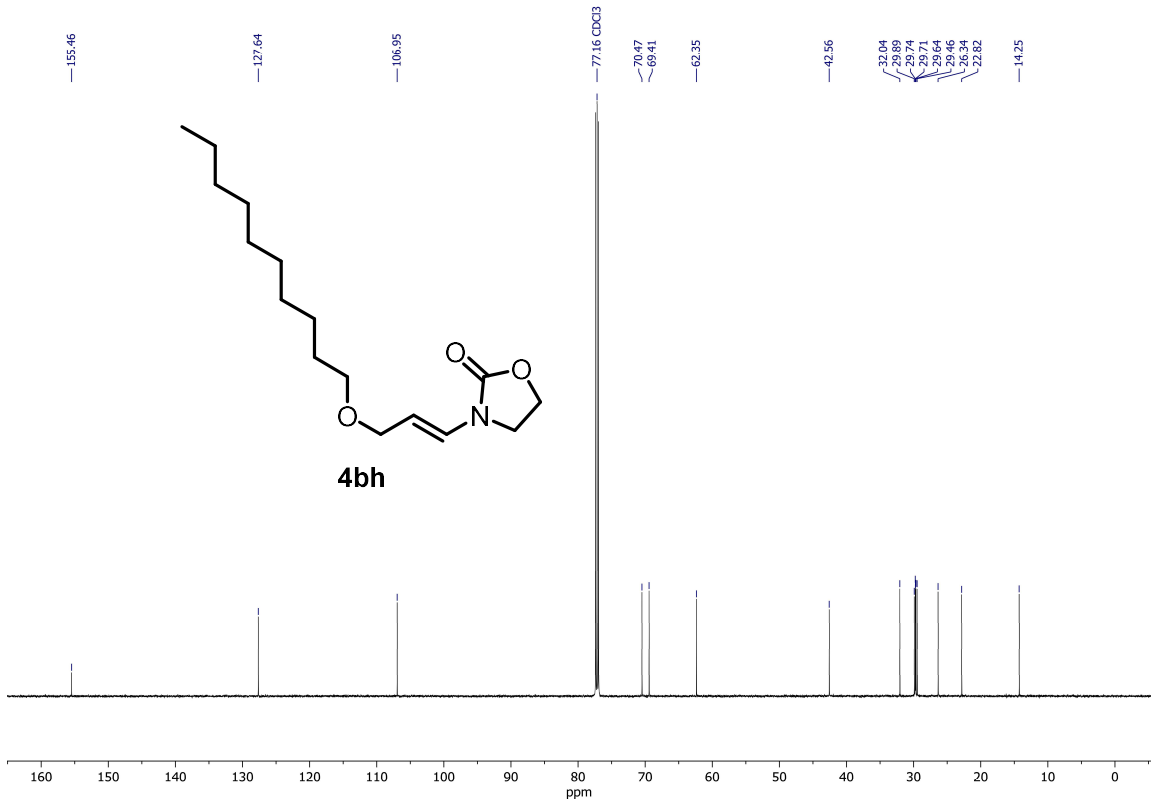
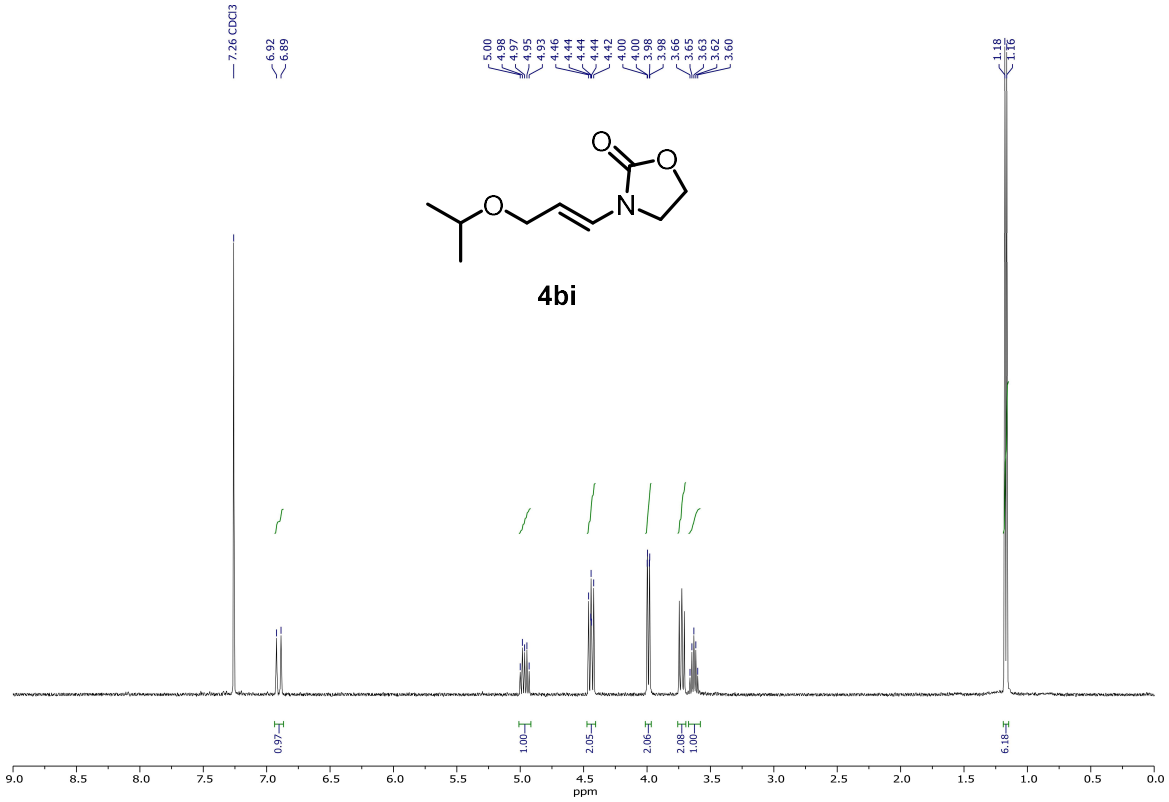
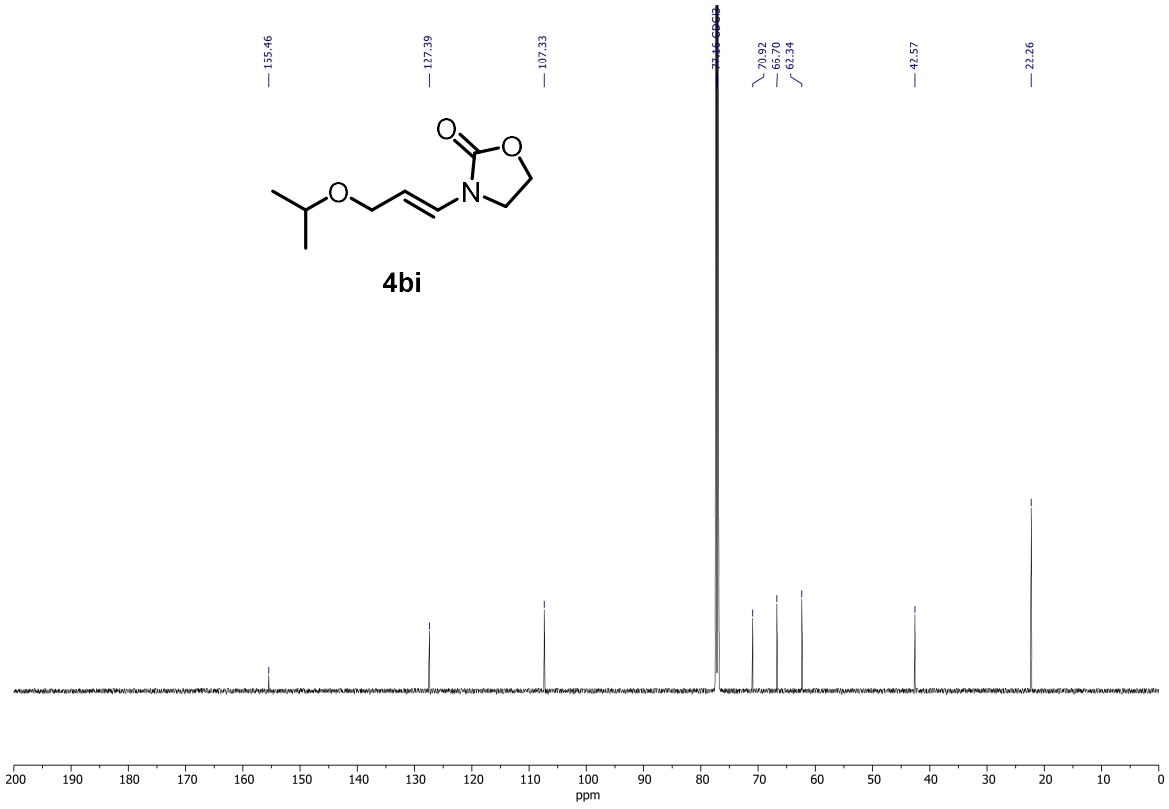


^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



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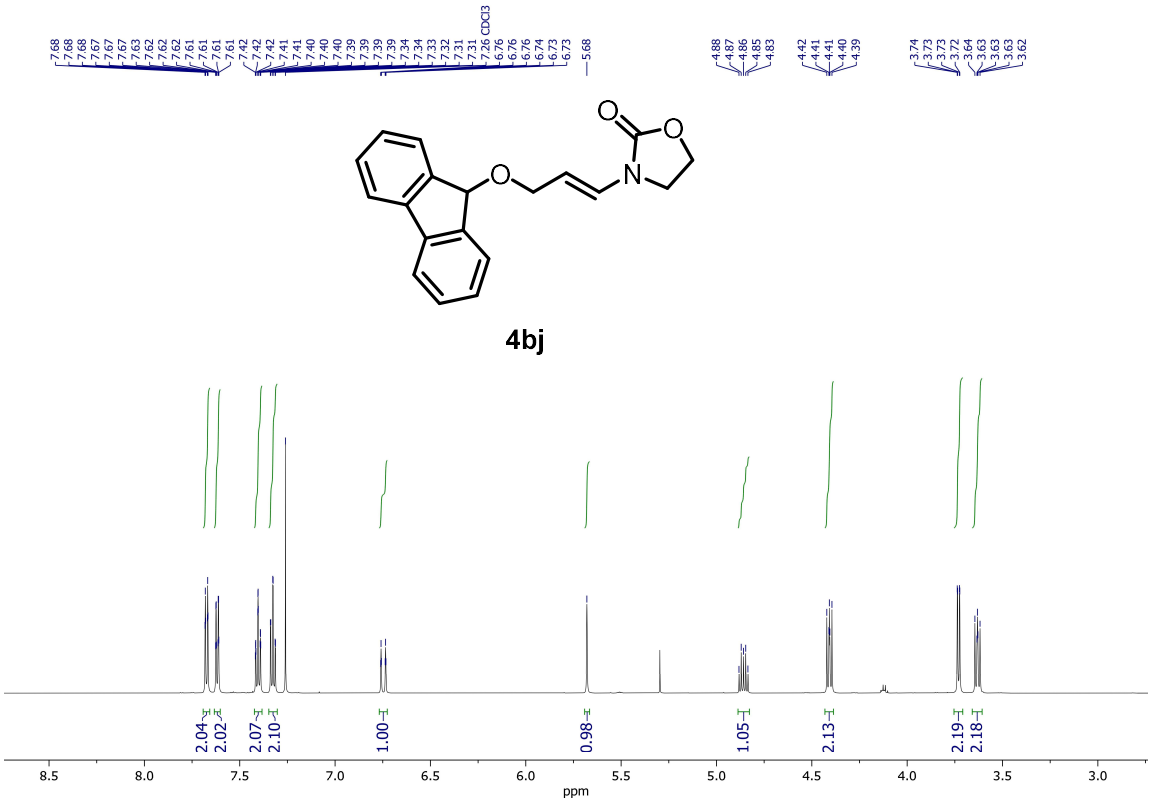
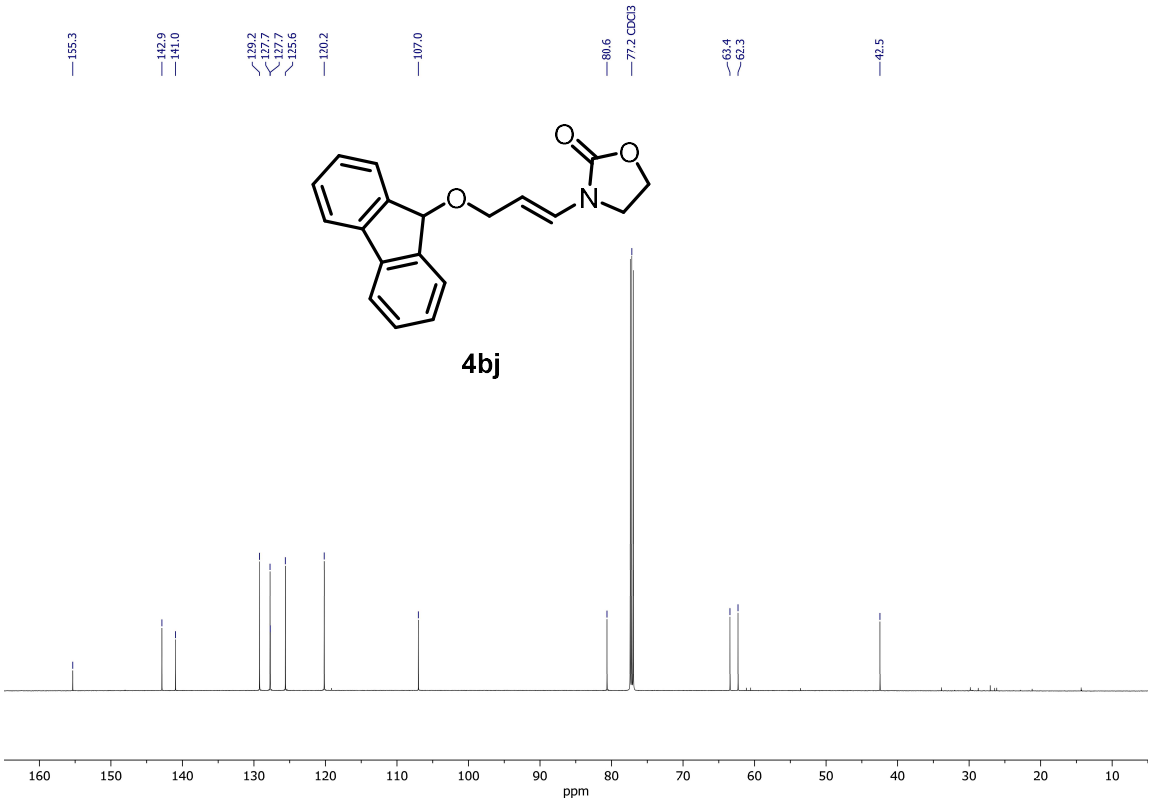
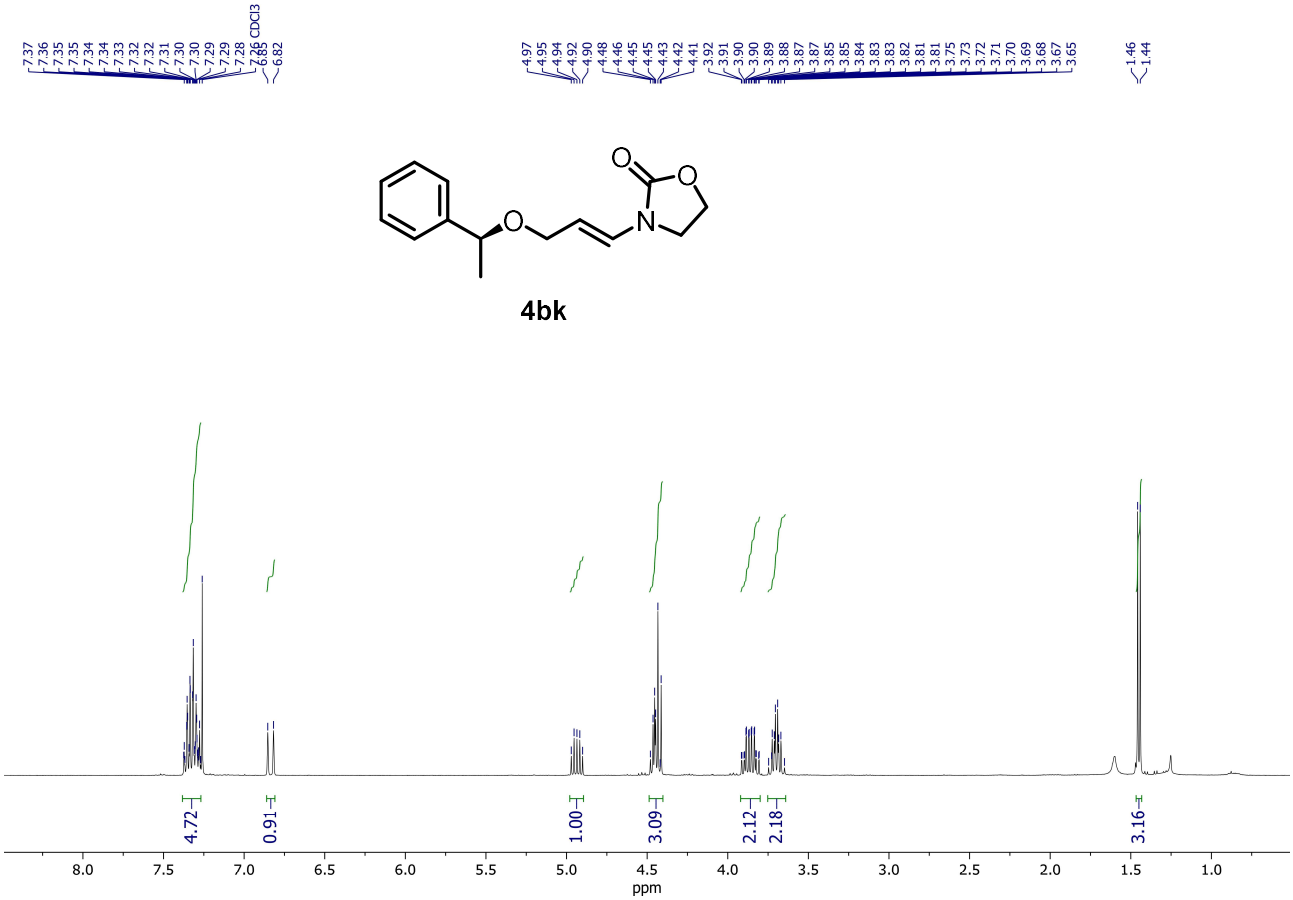


^{13}C NMR (150 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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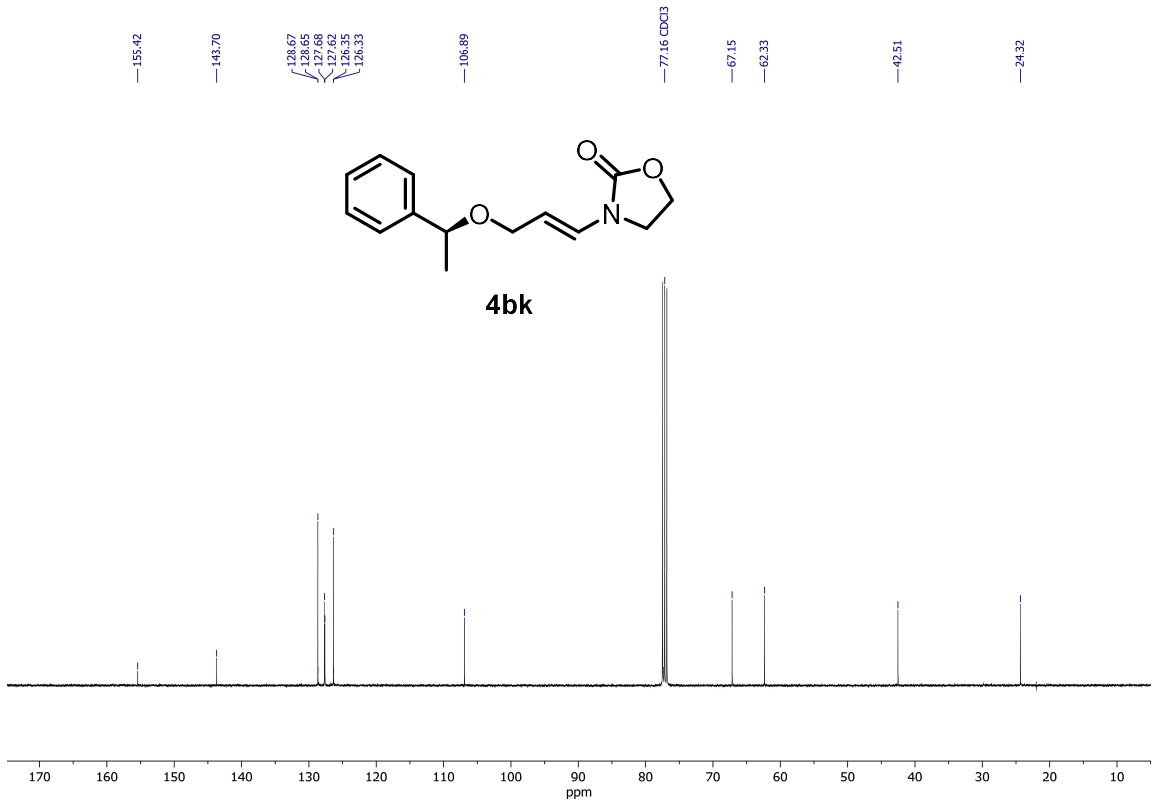

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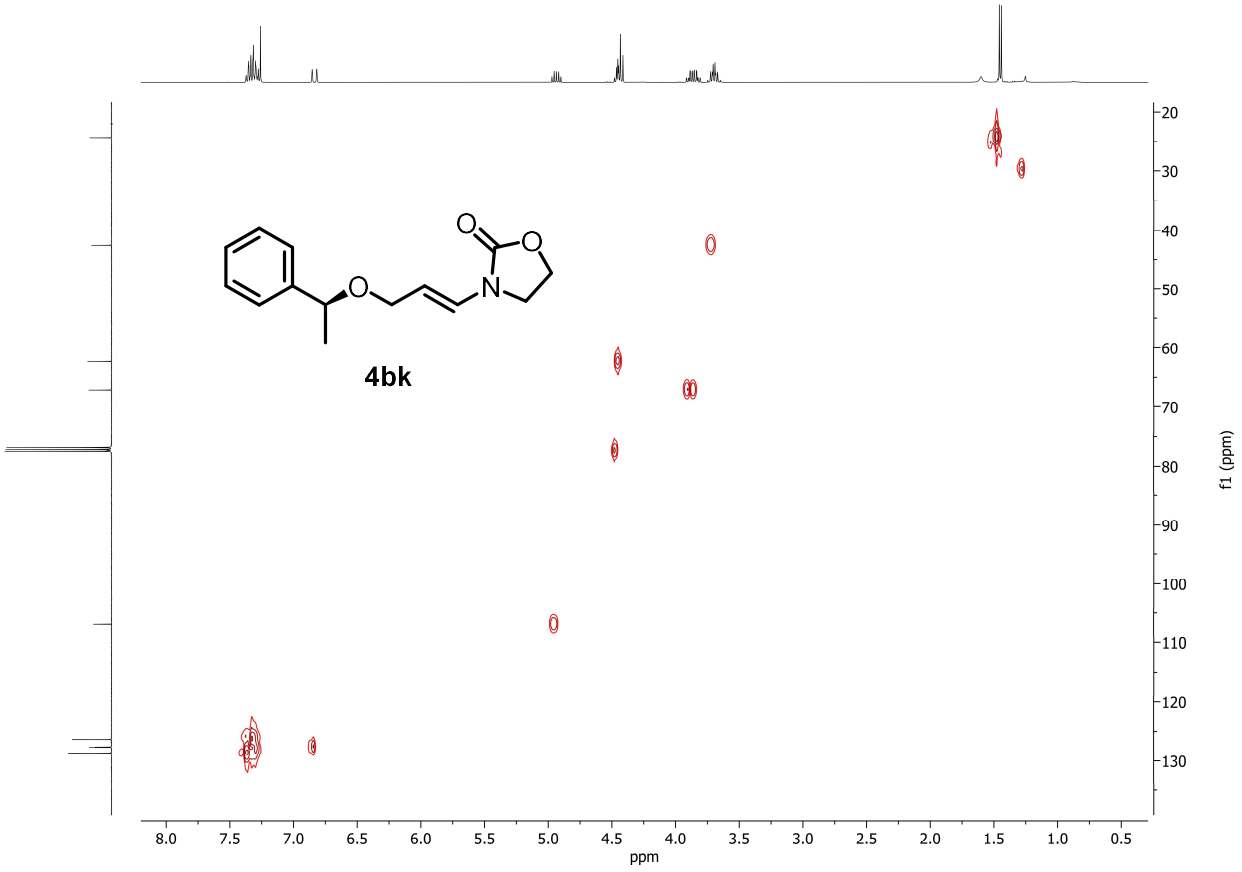
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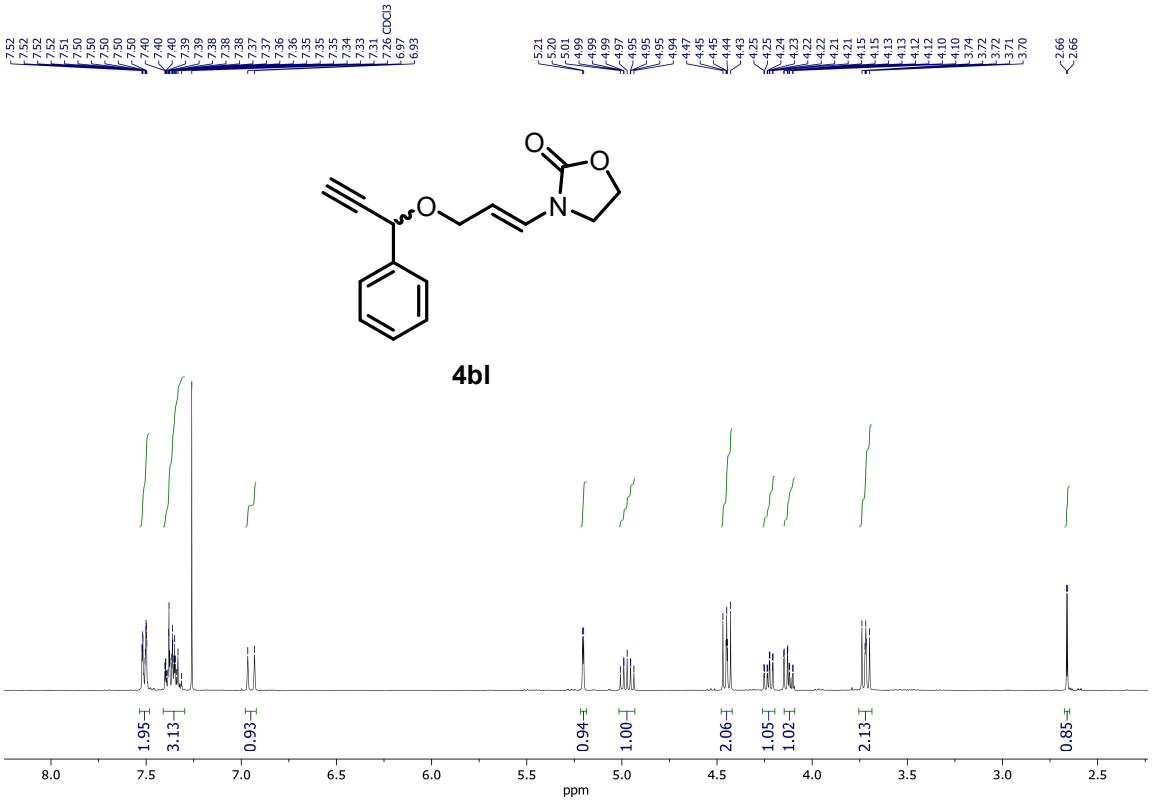
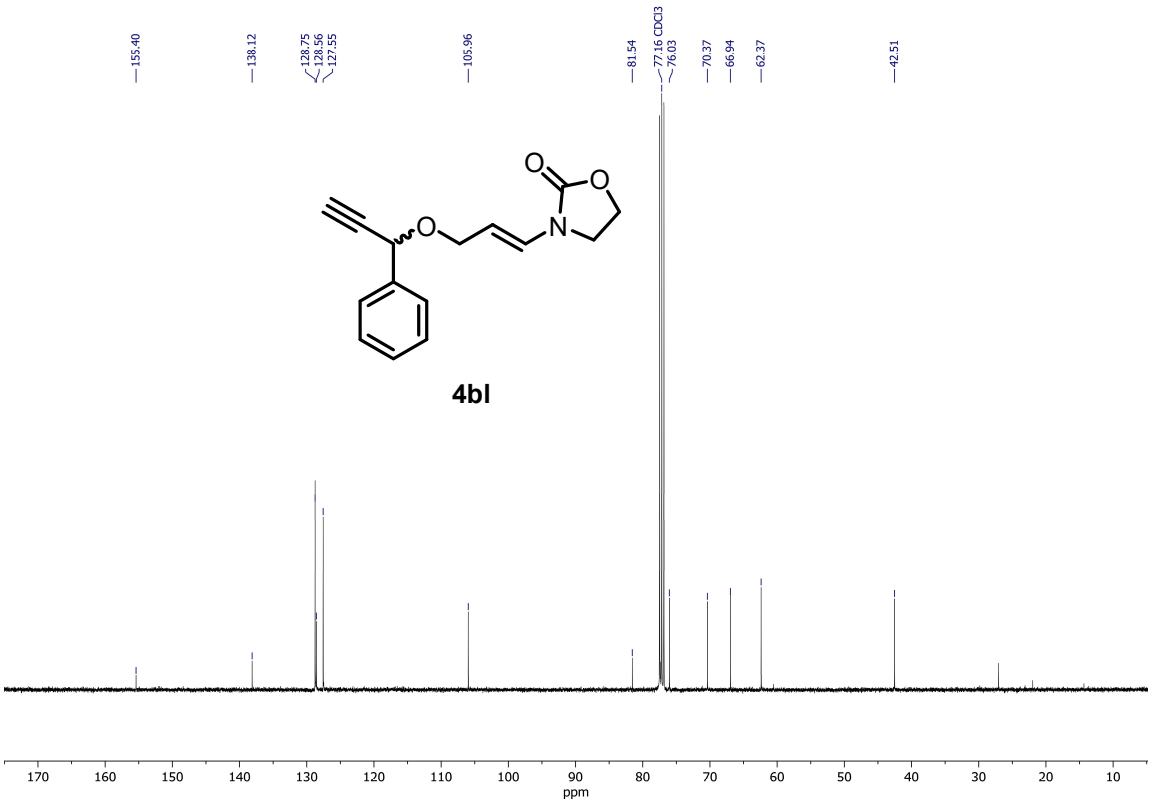
2.0
1.5
1.0
0.5
ppm
20
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)

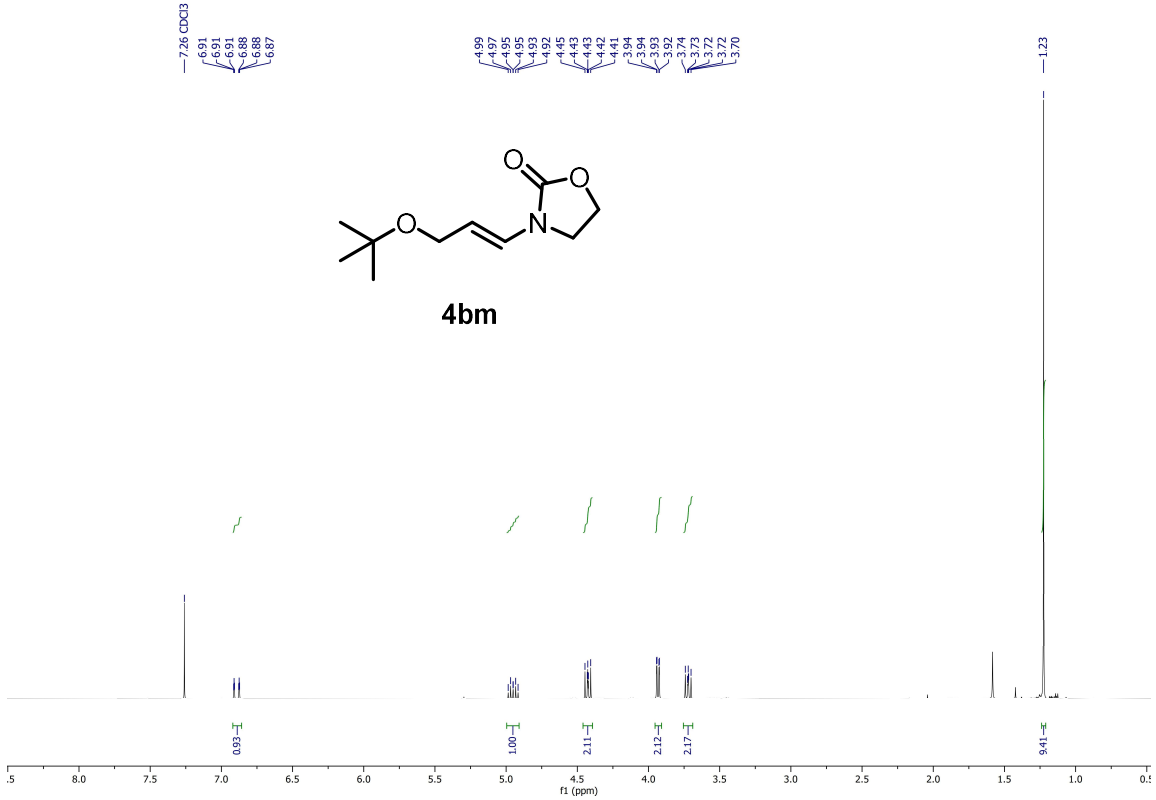
^{1}H NMR (400 MHz, $CDCl_3$)



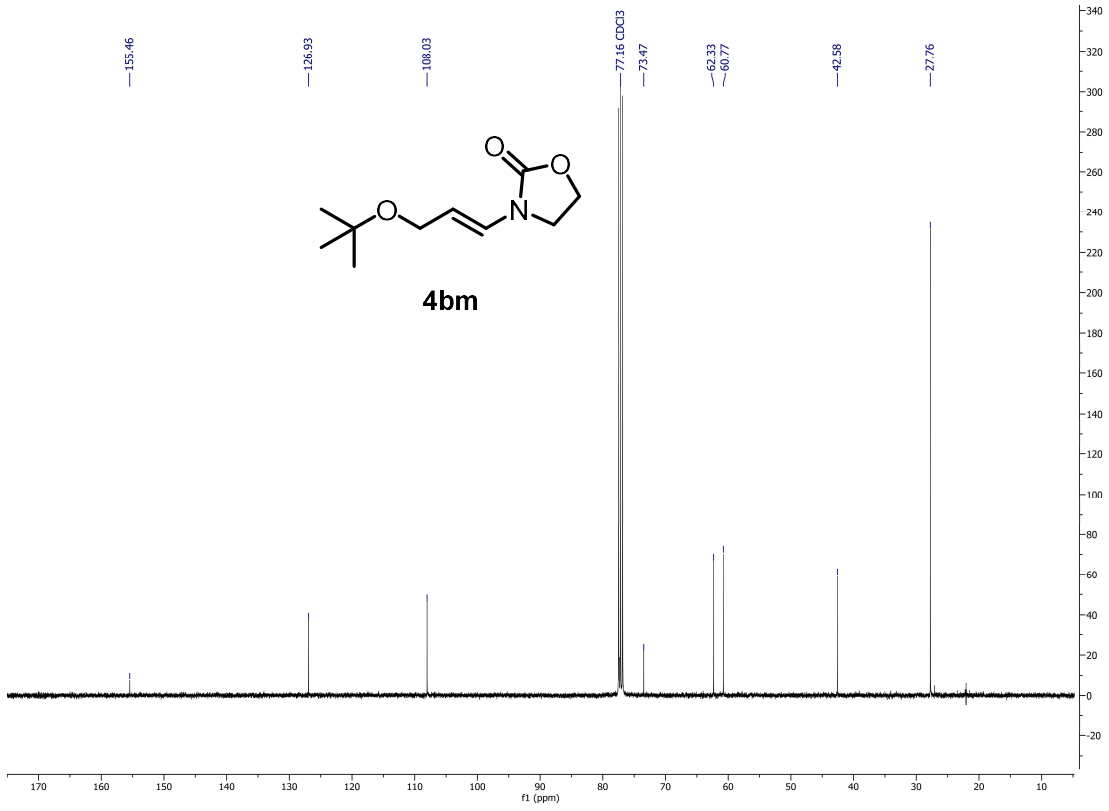
^{13}C NMR (100 MHz, $CDCl_3$)



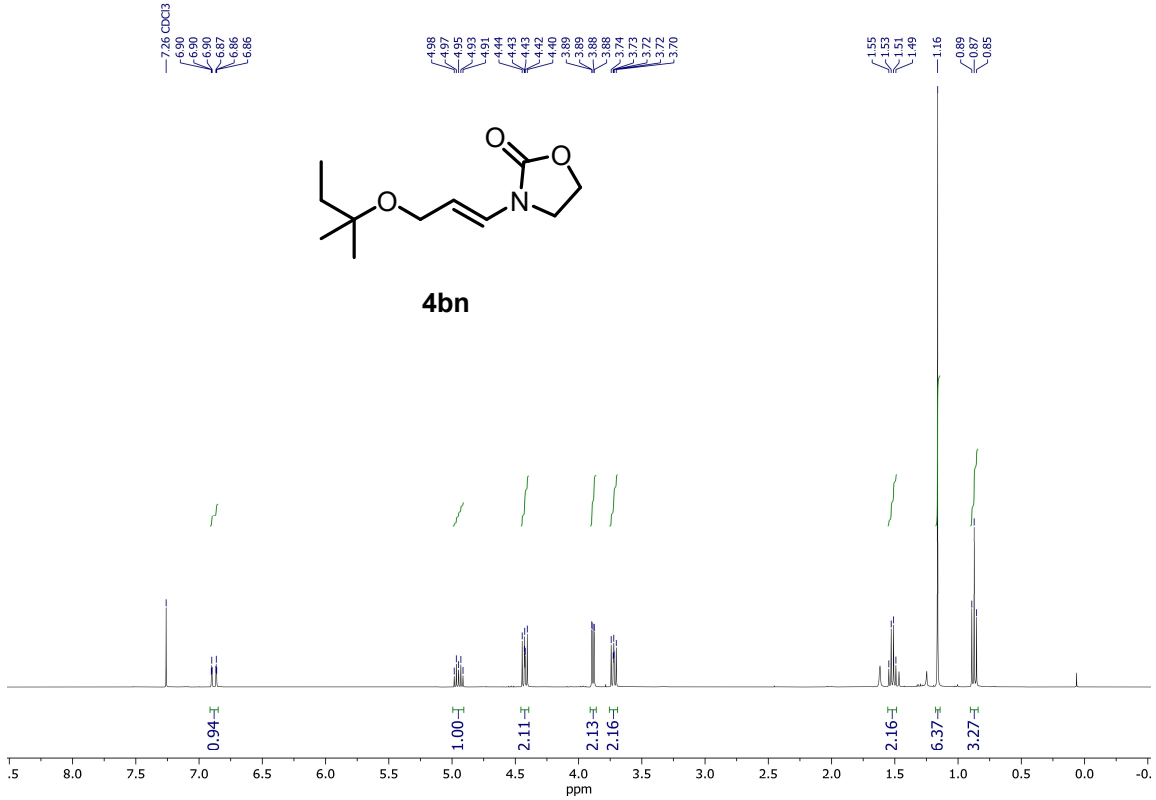
^{1}H NMR (400 MHz, $CDCl_3$)



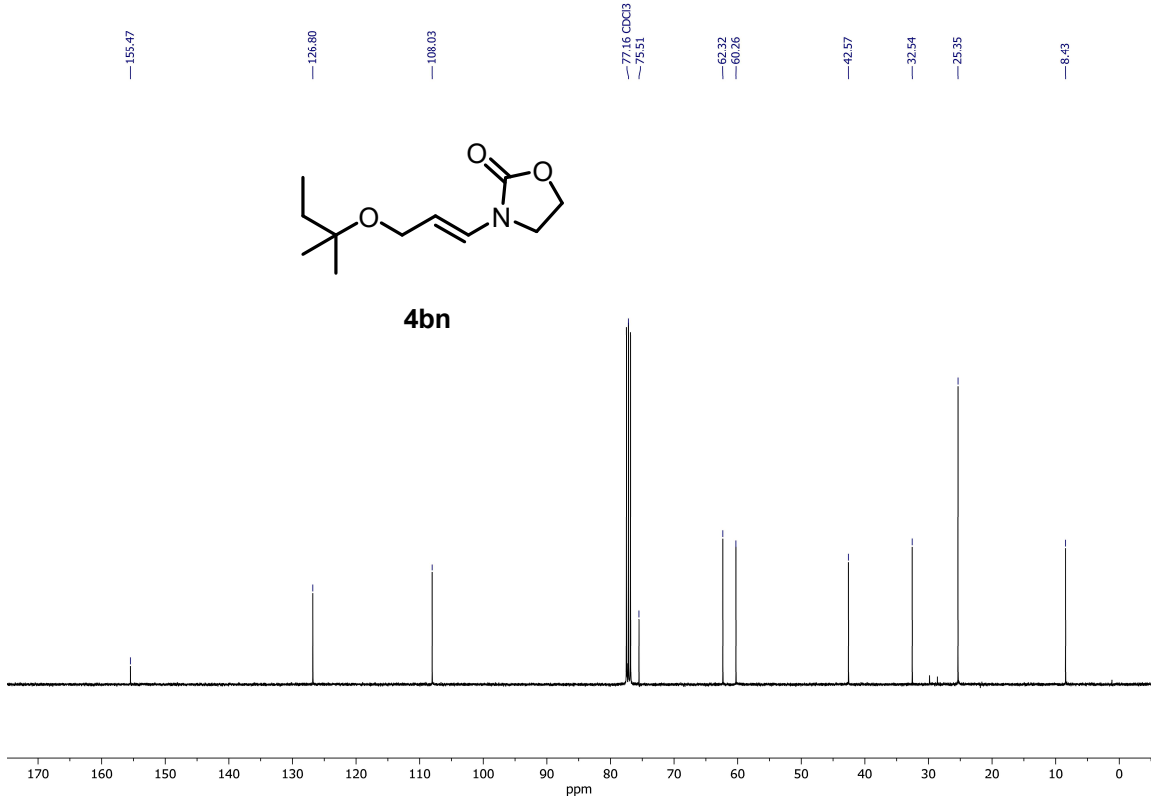
^{13}C NMR (100 MHz, $CDCl_3$)



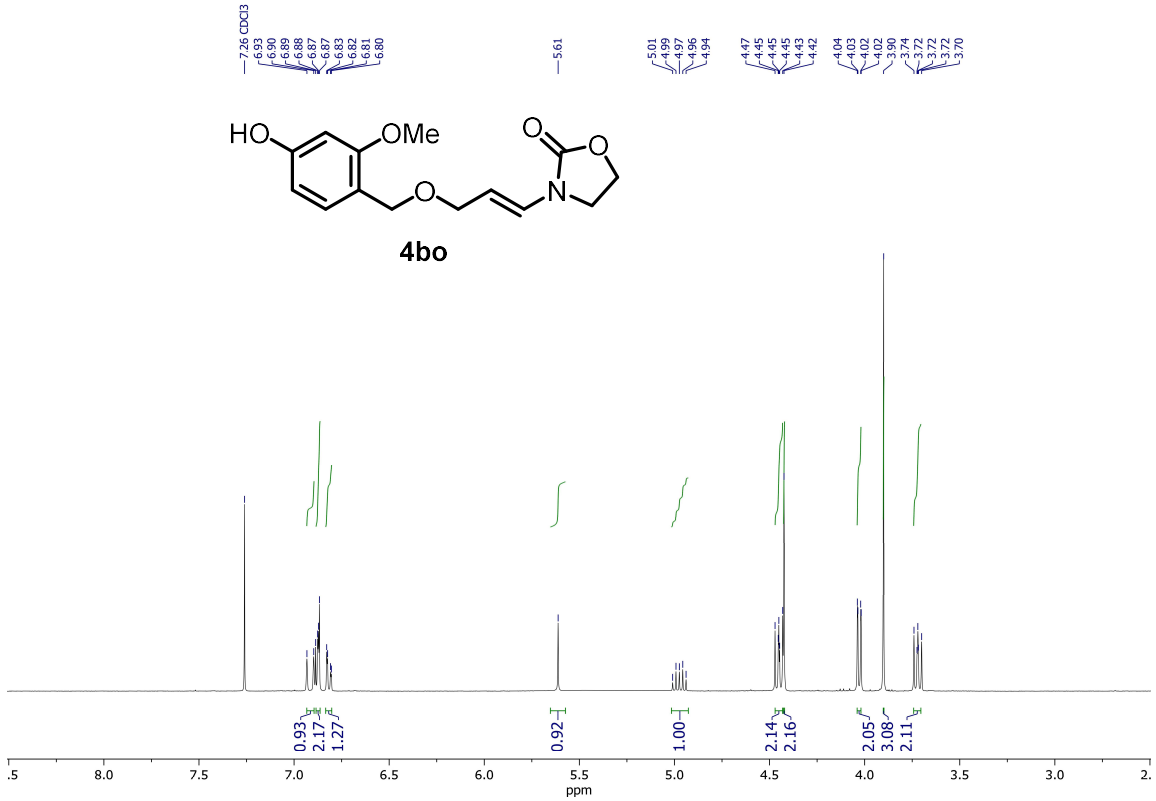
^{1}H NMR (400 MHz, $CDCl_3$)



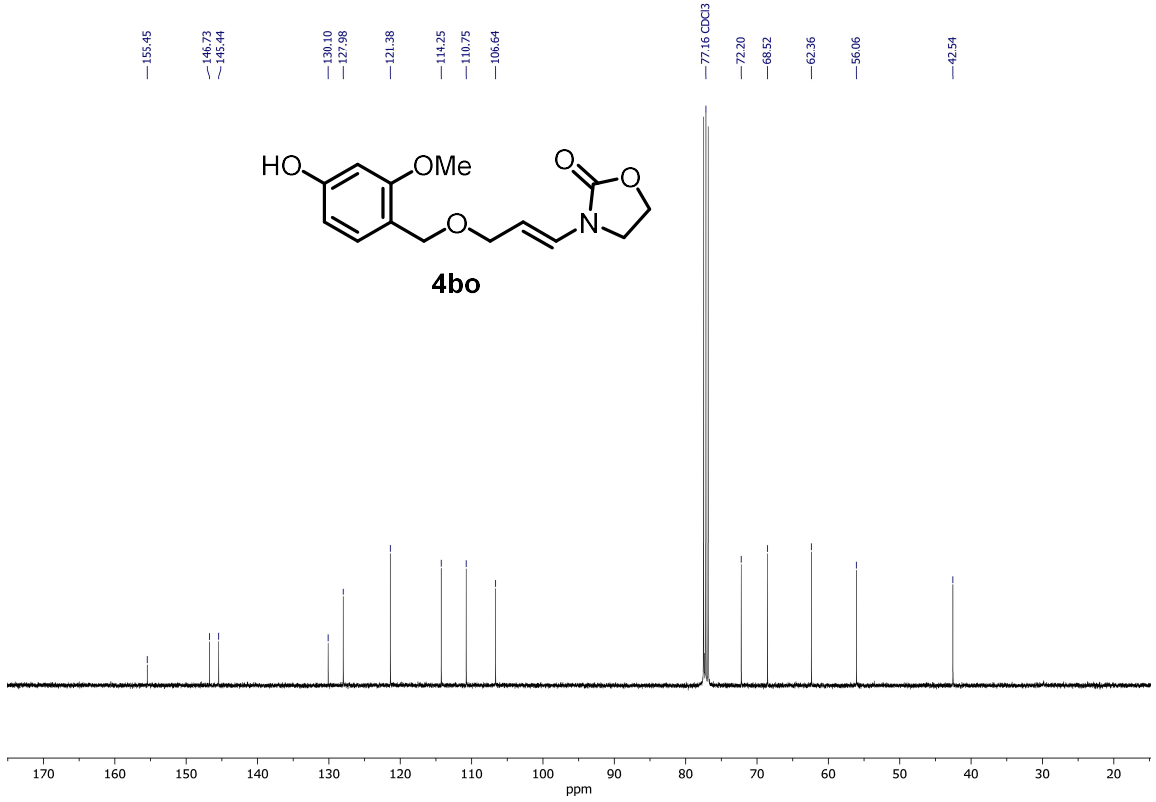
^{13}C NMR (100 MHz, $CDCl_3$)



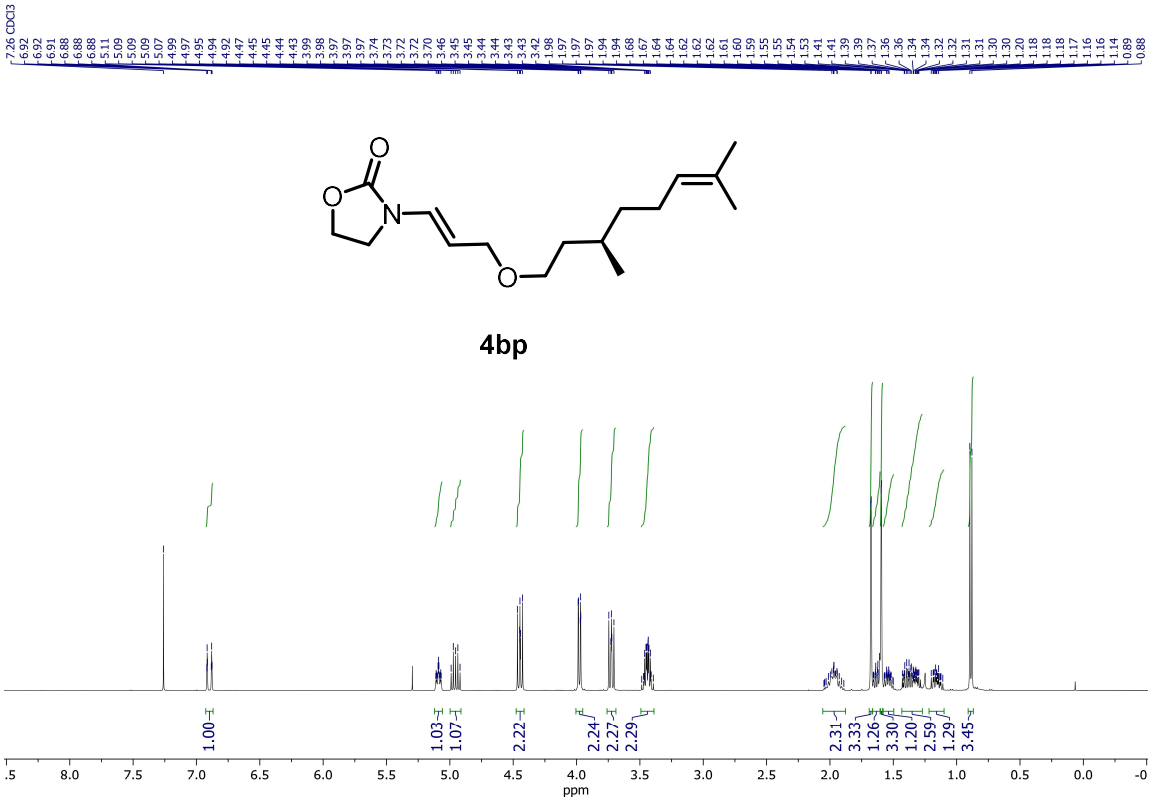
^{1}H NMR (400 MHz, $CDCl_3$)



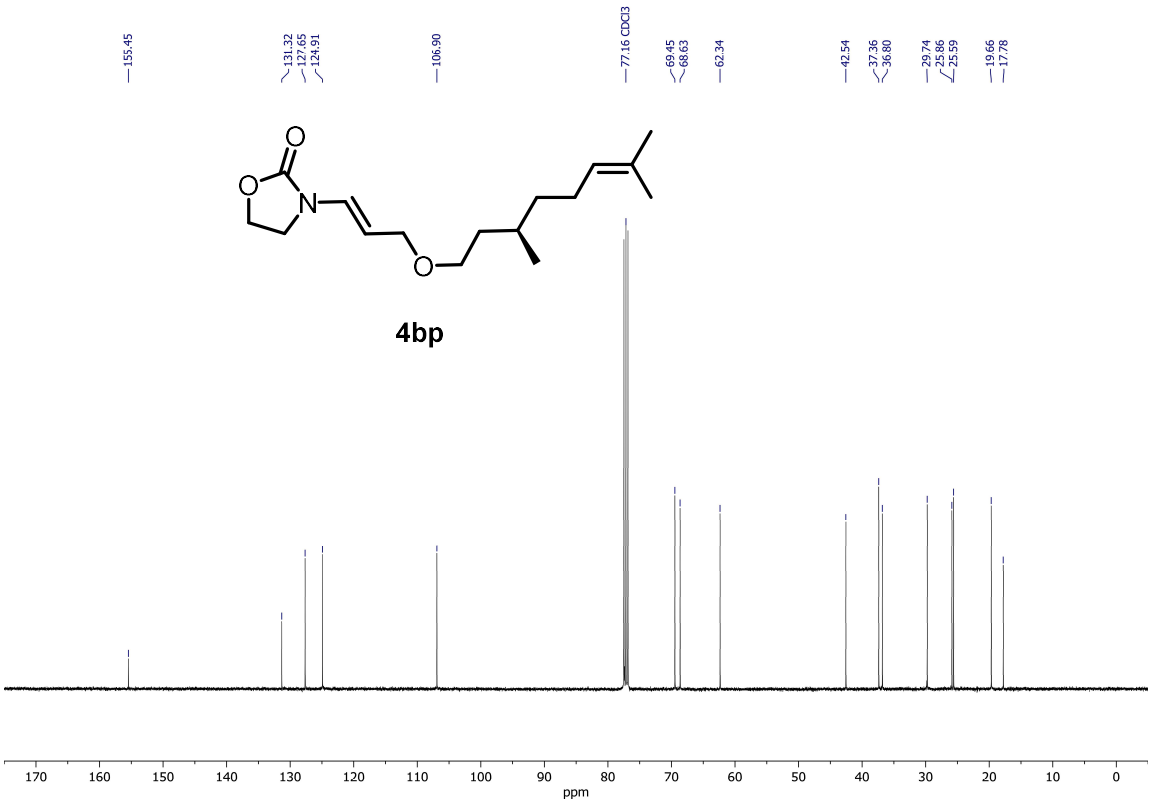
^{13}C NMR (100 MHz, $CDCl_3$)



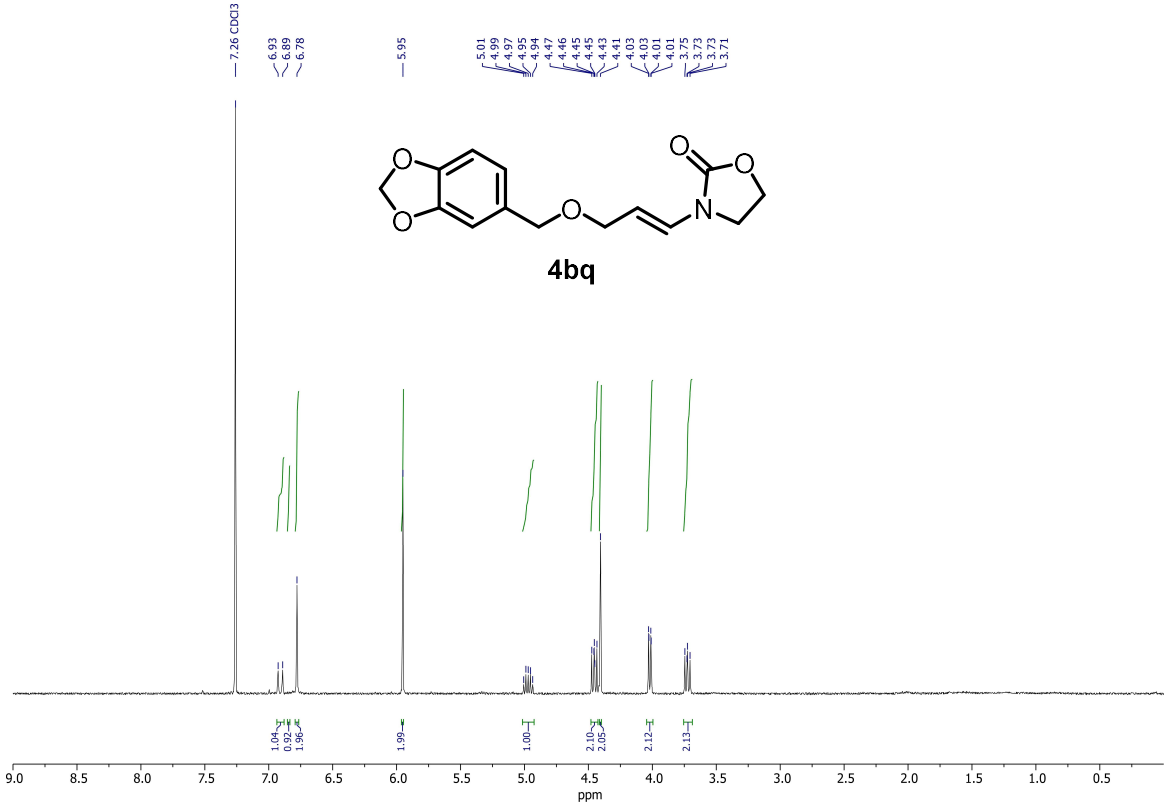
^{1}H NMR (400 MHz, $CDCl_3$)



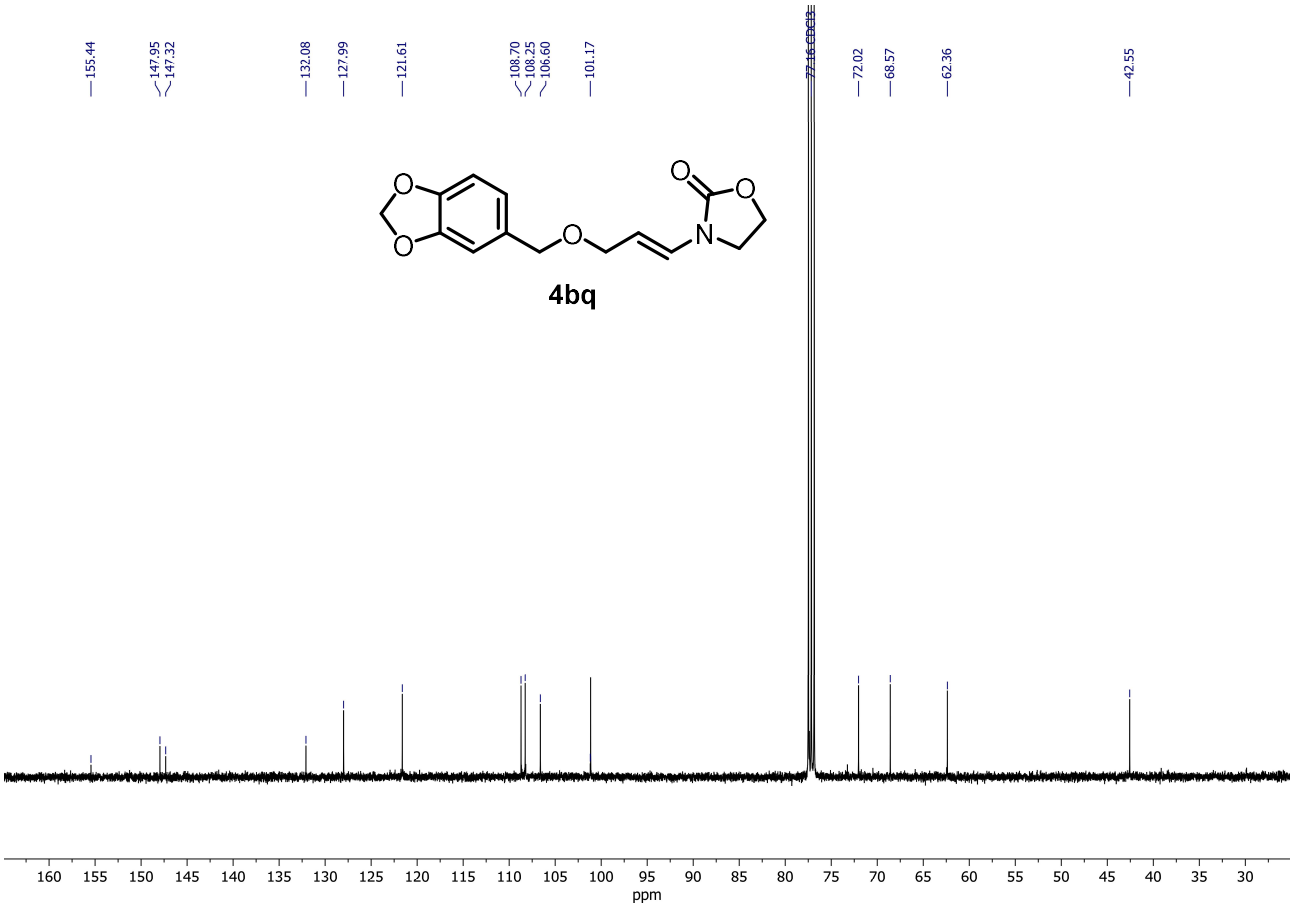
^{13}C NMR (100 MHz, $CDCl_3$)



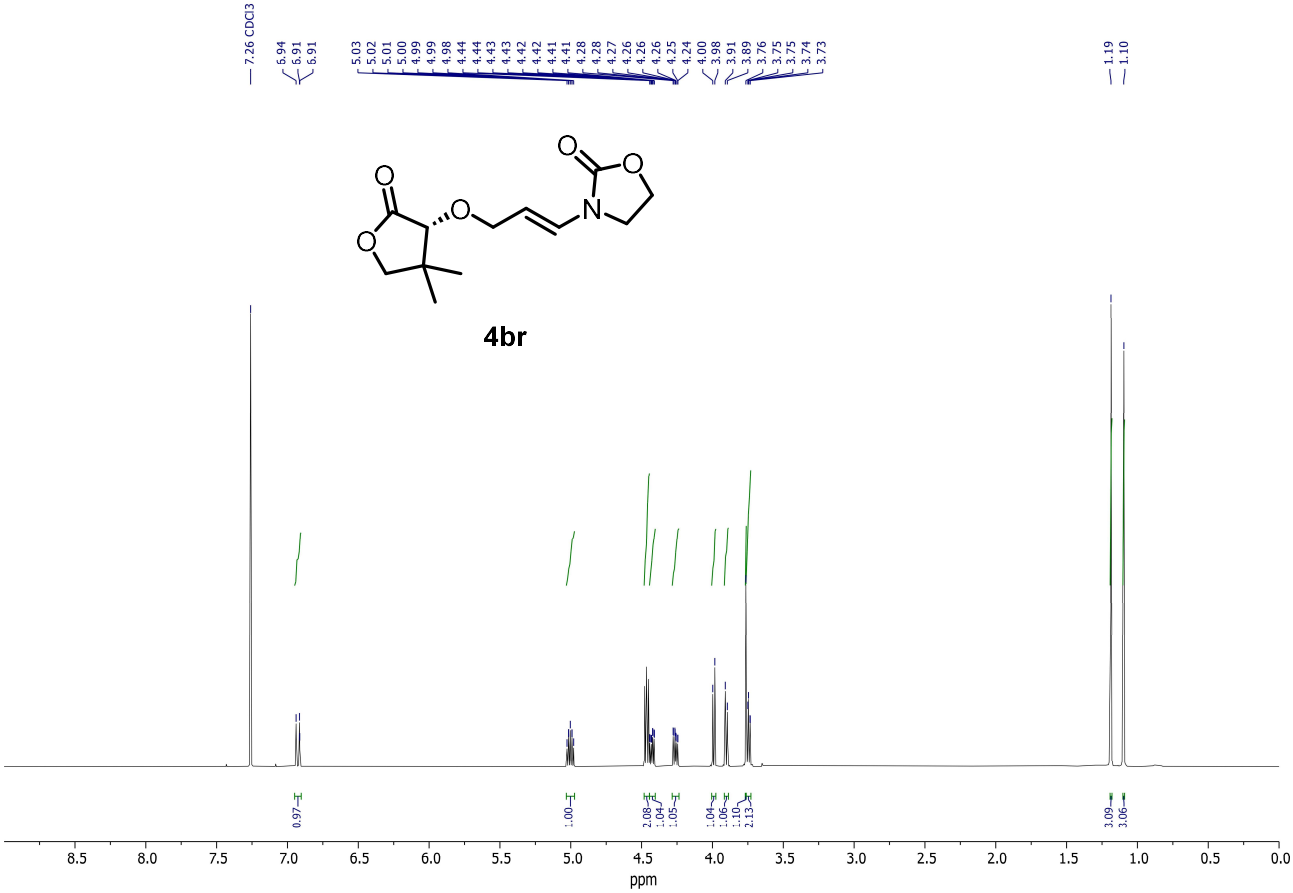
^{1}H NMR (400 MHz, $CDCl_3$)



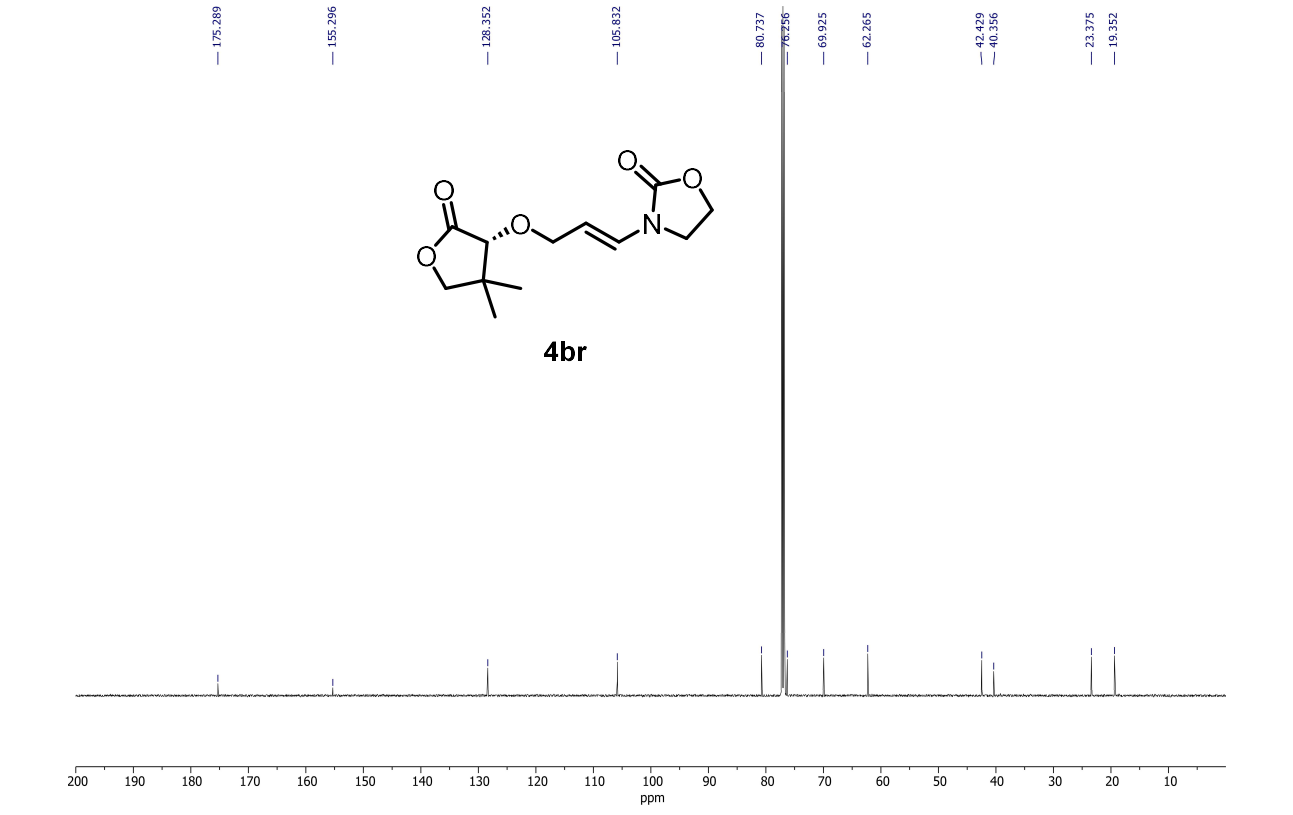
^{13}C NMR (100 MHz, $CDCl_3$)



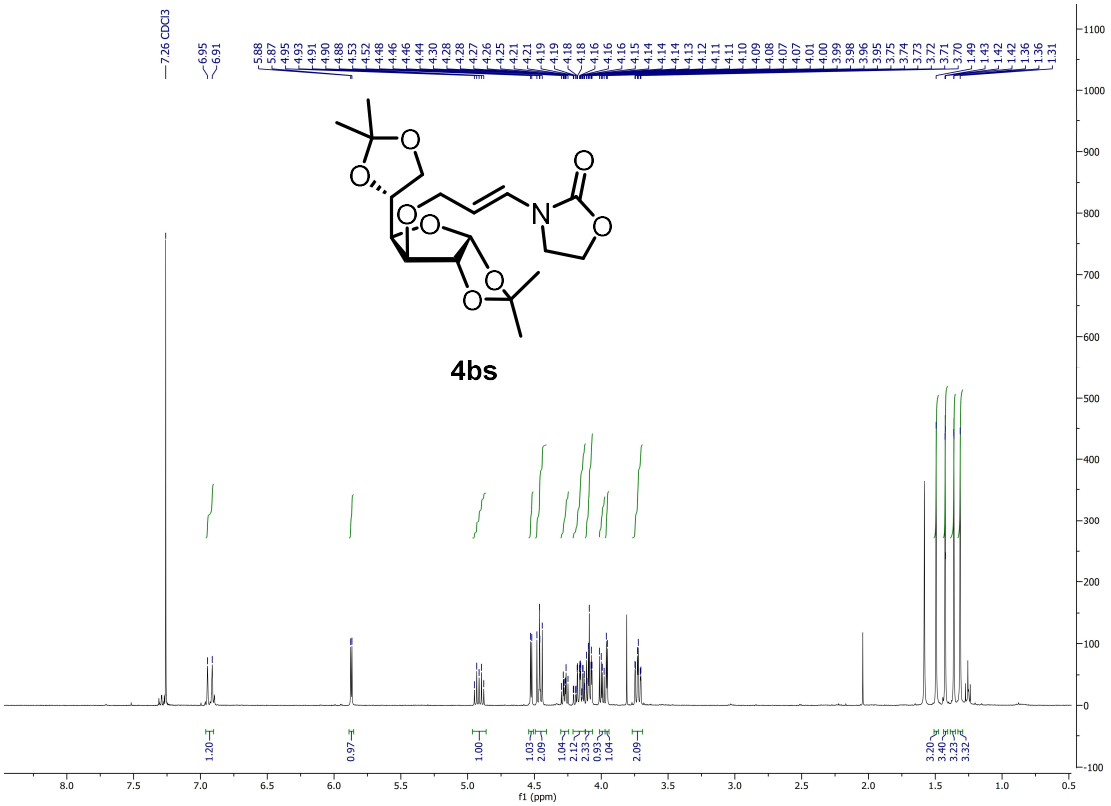
^{1}H NMR (600 MHz, $CDCl_3$)



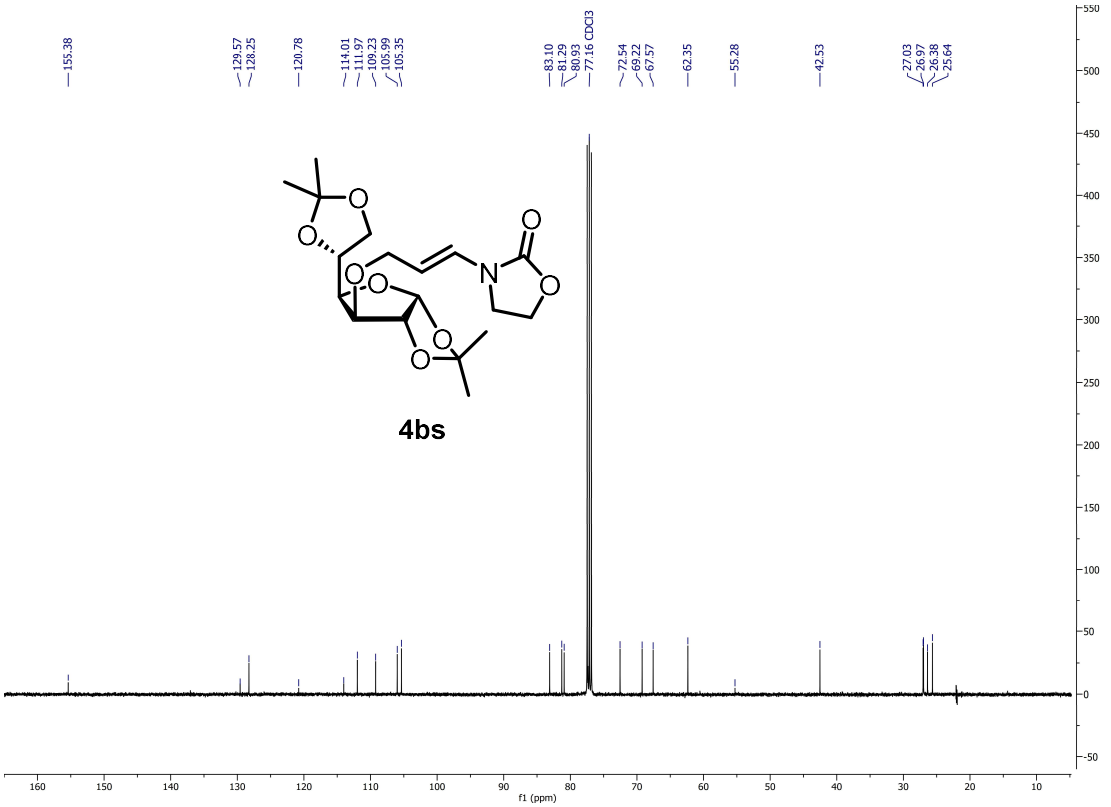
^{13}C NMR (150 MHz, $CDCl_3$)



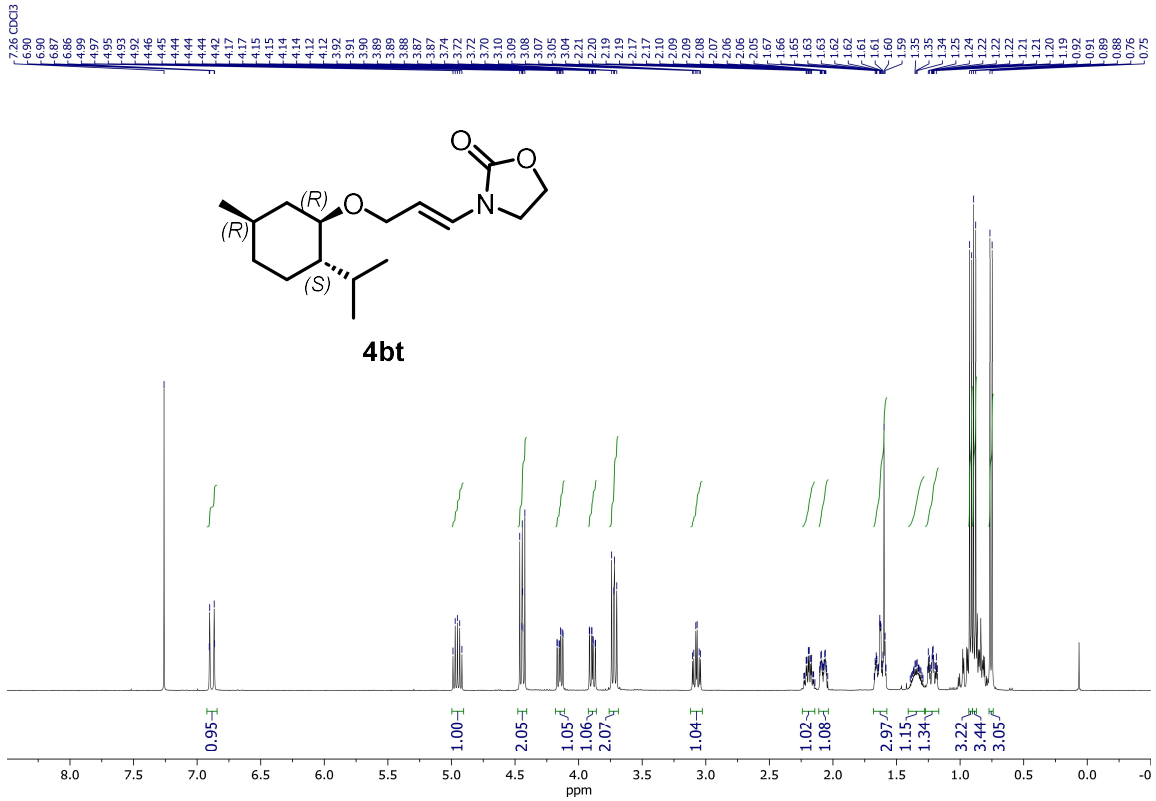
^{1}H NMR (400 MHz, $CDCl_3$)



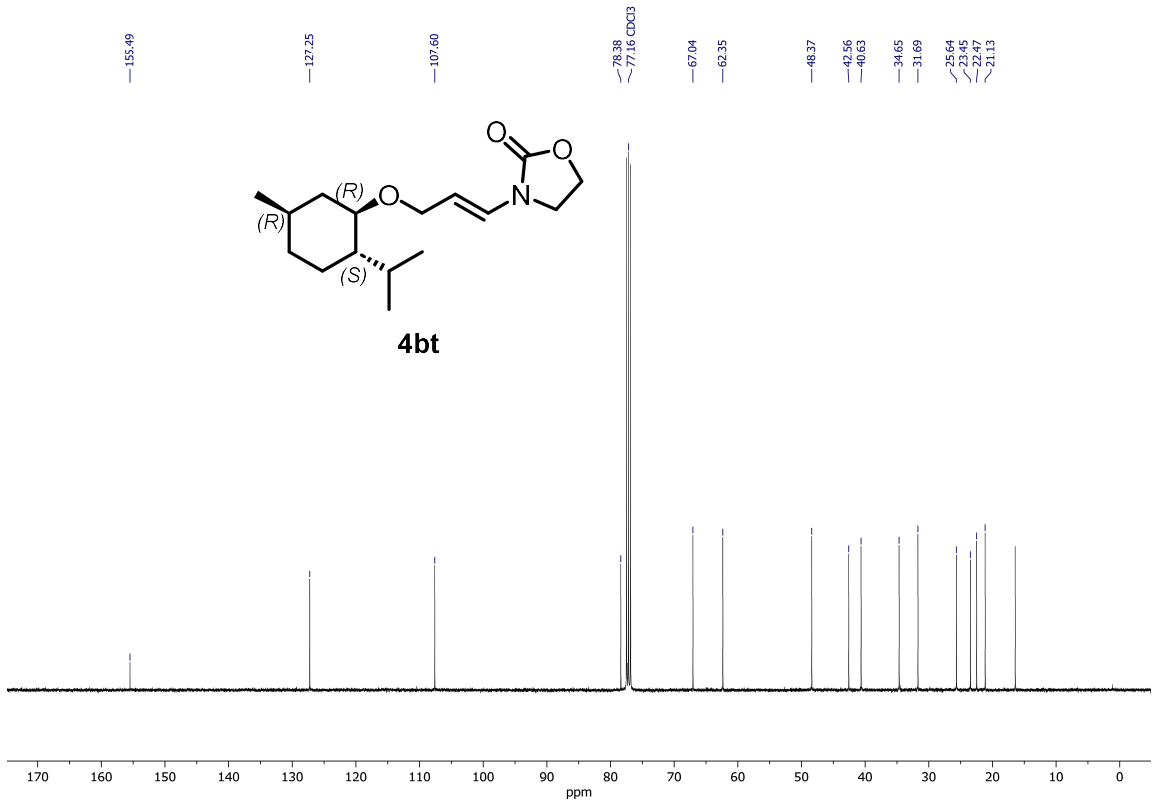
^{13}C NMR (100 MHz, $CDCl_3$)



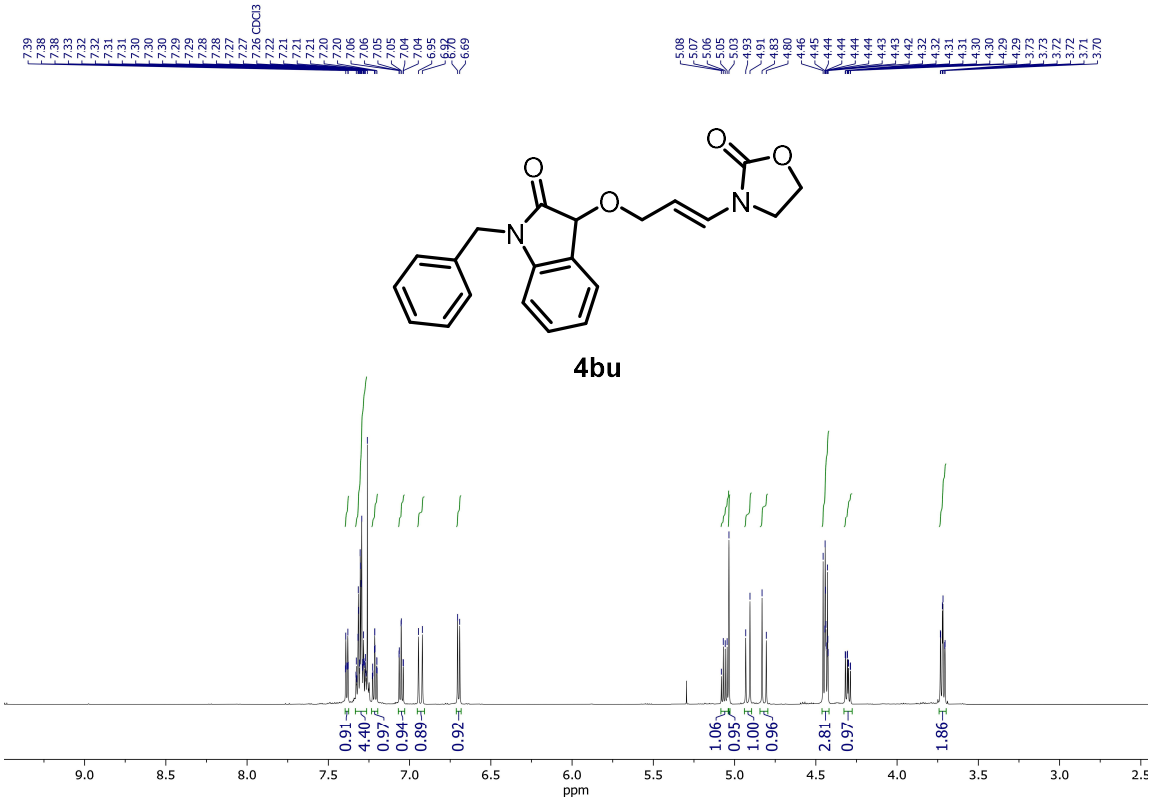
^{1}H NMR (400 MHz, $CDCl_3$)



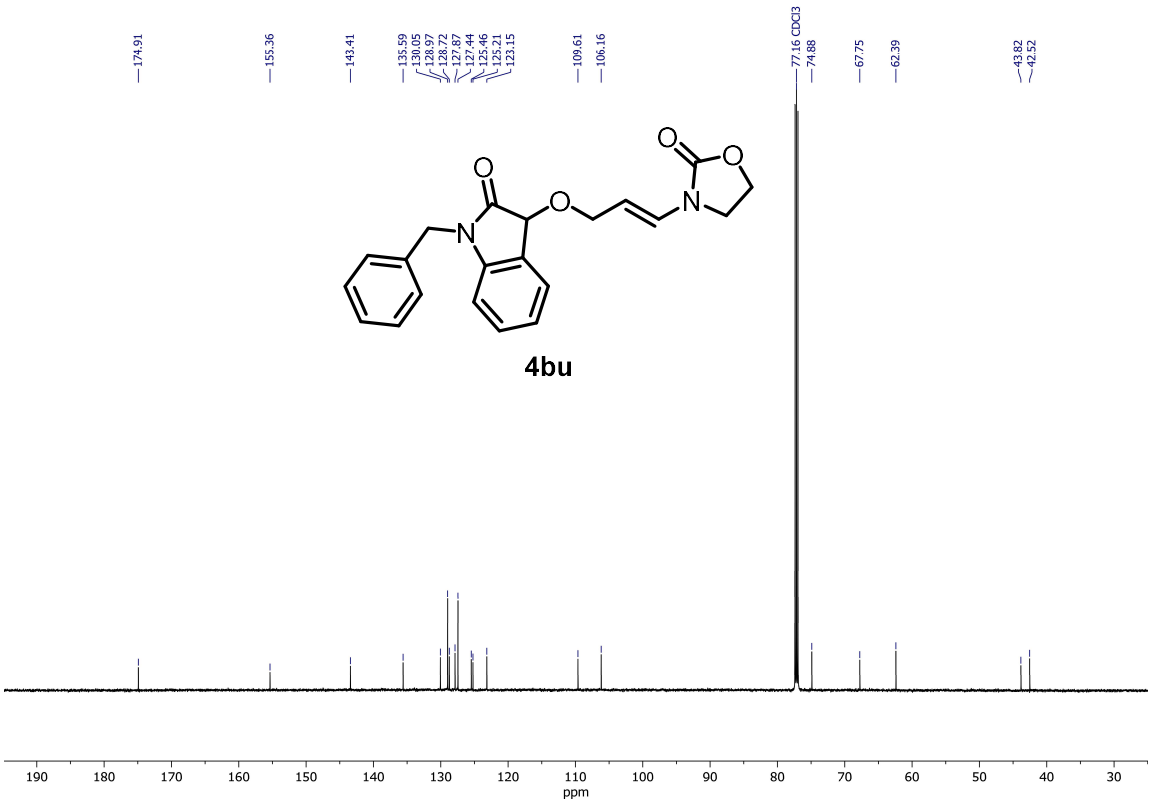
^{13}C NMR (100 MHz, $CDCl_3$)



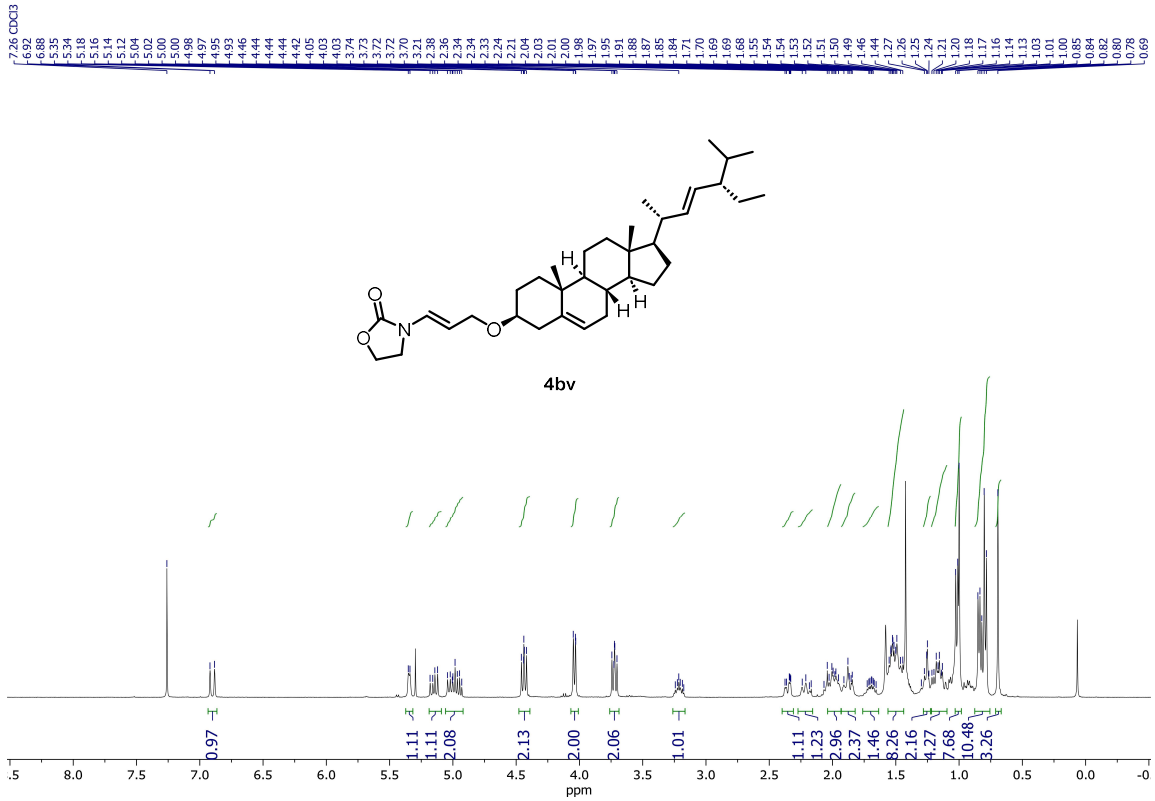
^{1}H NMR (600 MHz, $CDCl_3$)



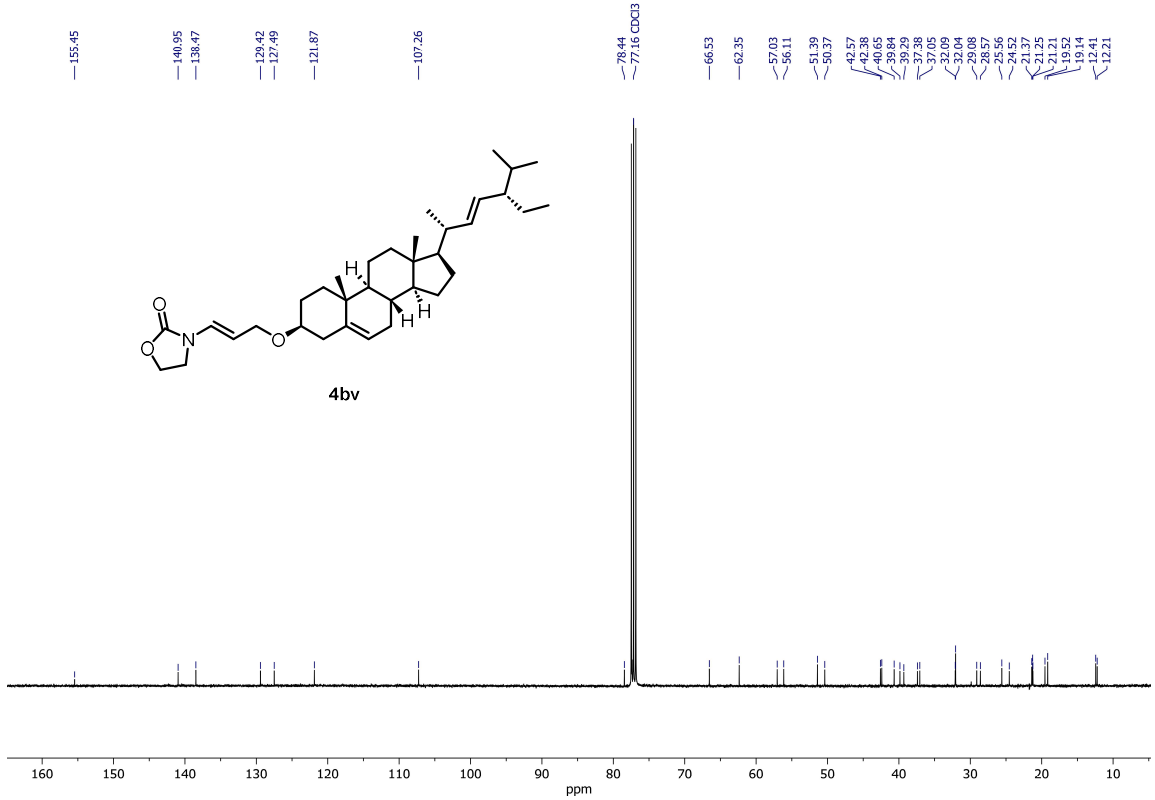
^{13}C NMR (150 MHz, $CDCl_3$)



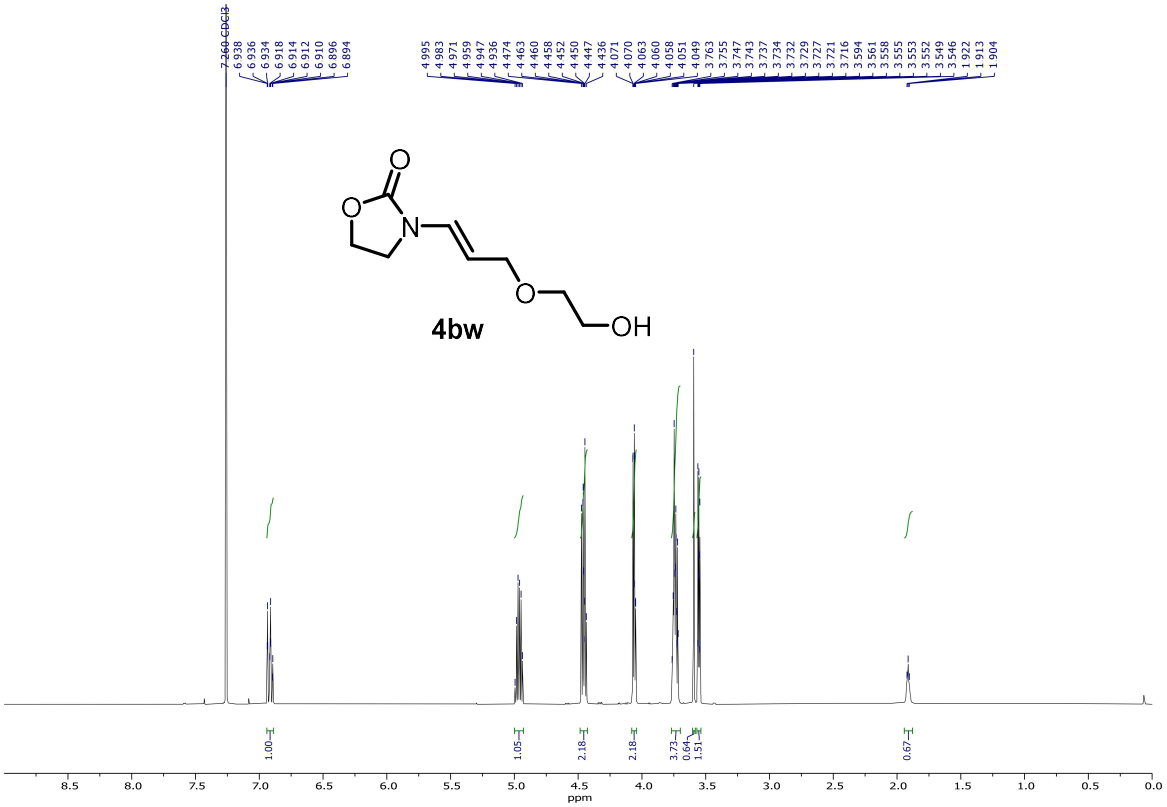
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (600 MHz, $CDCl_3$)



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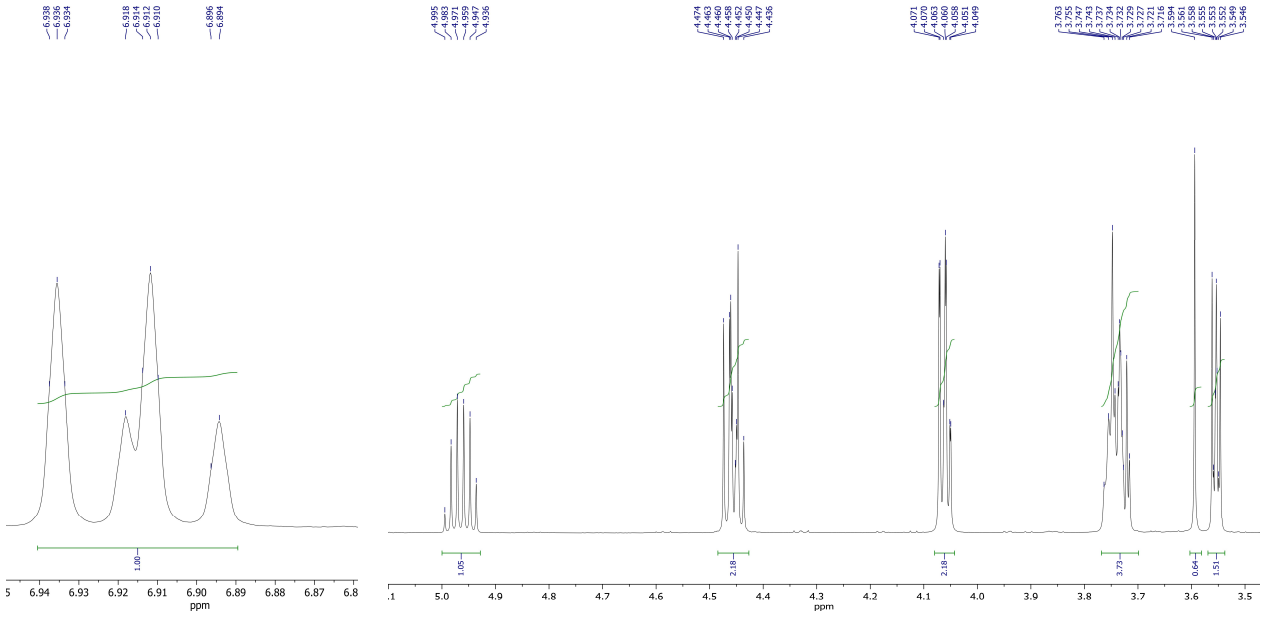
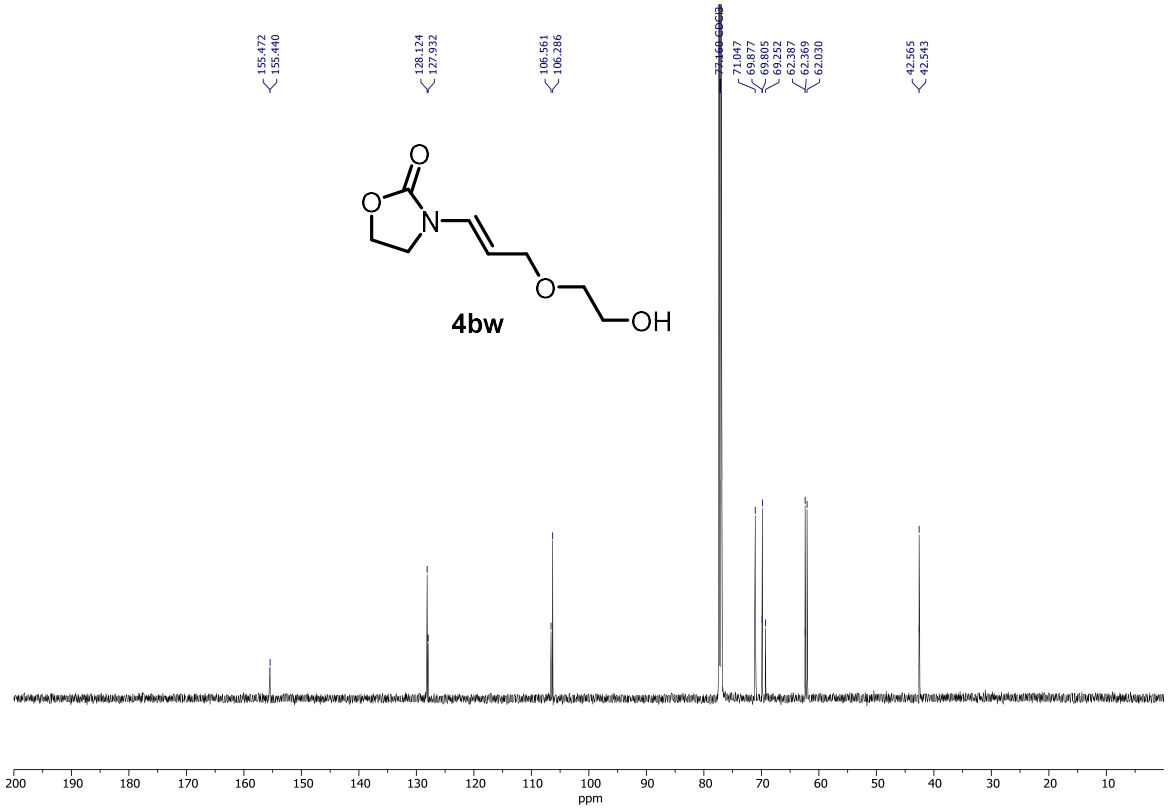
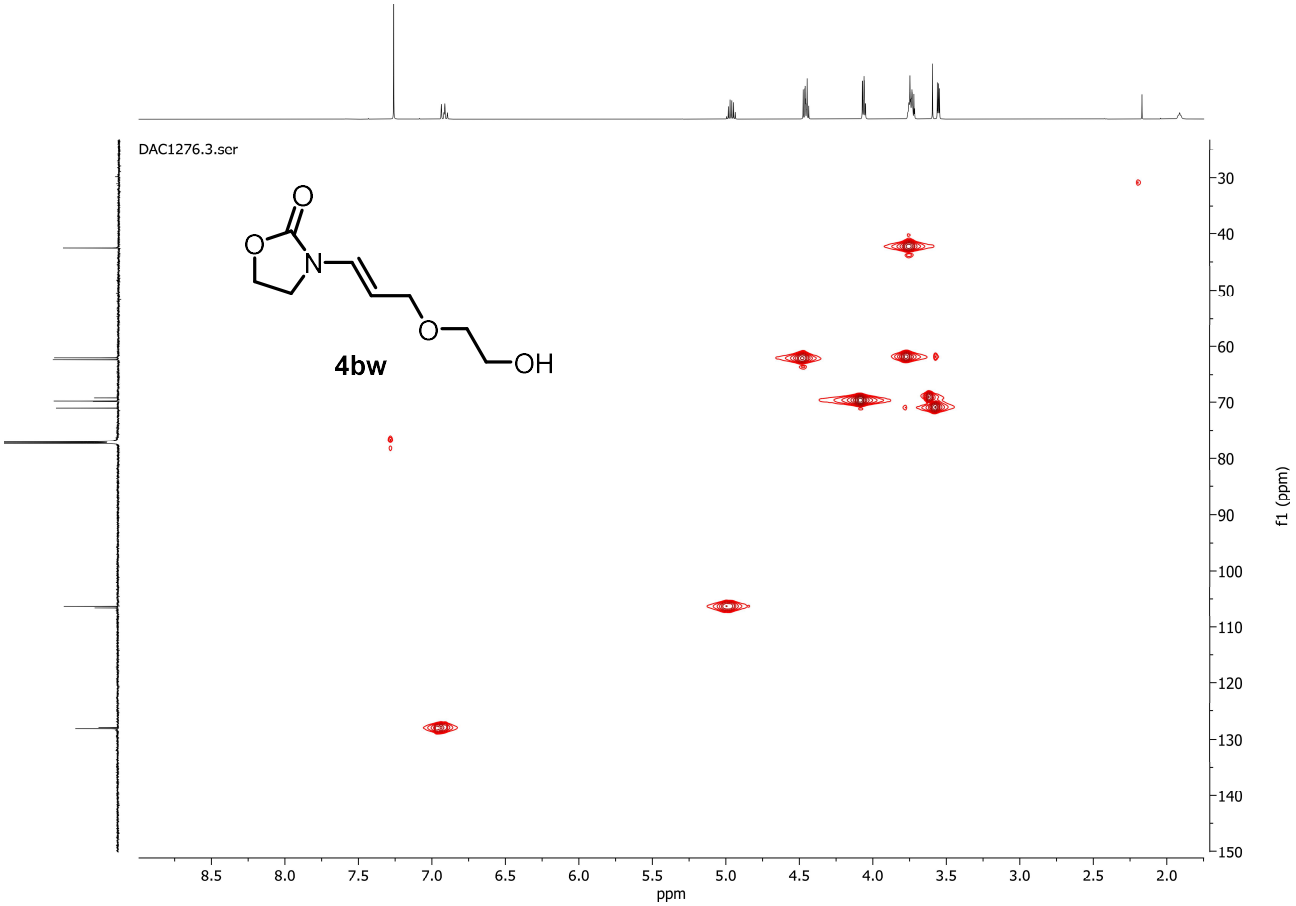


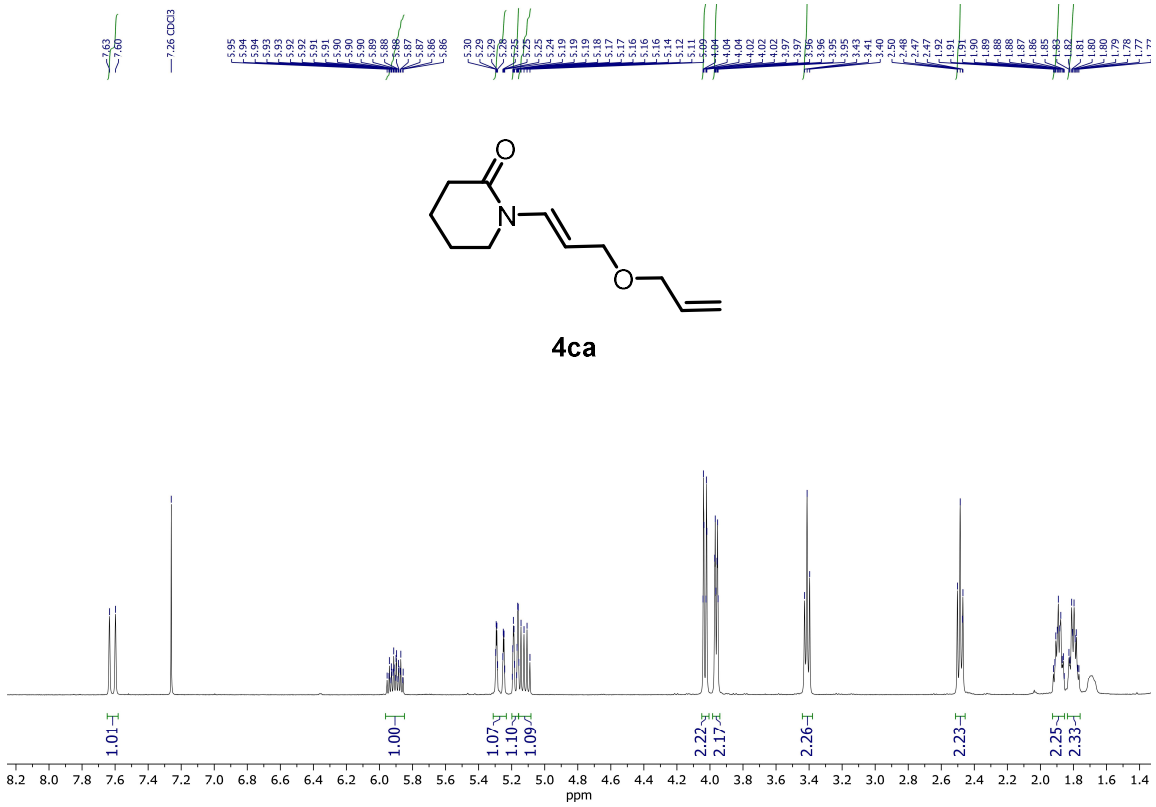
^{13}C NMR (150 MHz, $CDCl_3$)



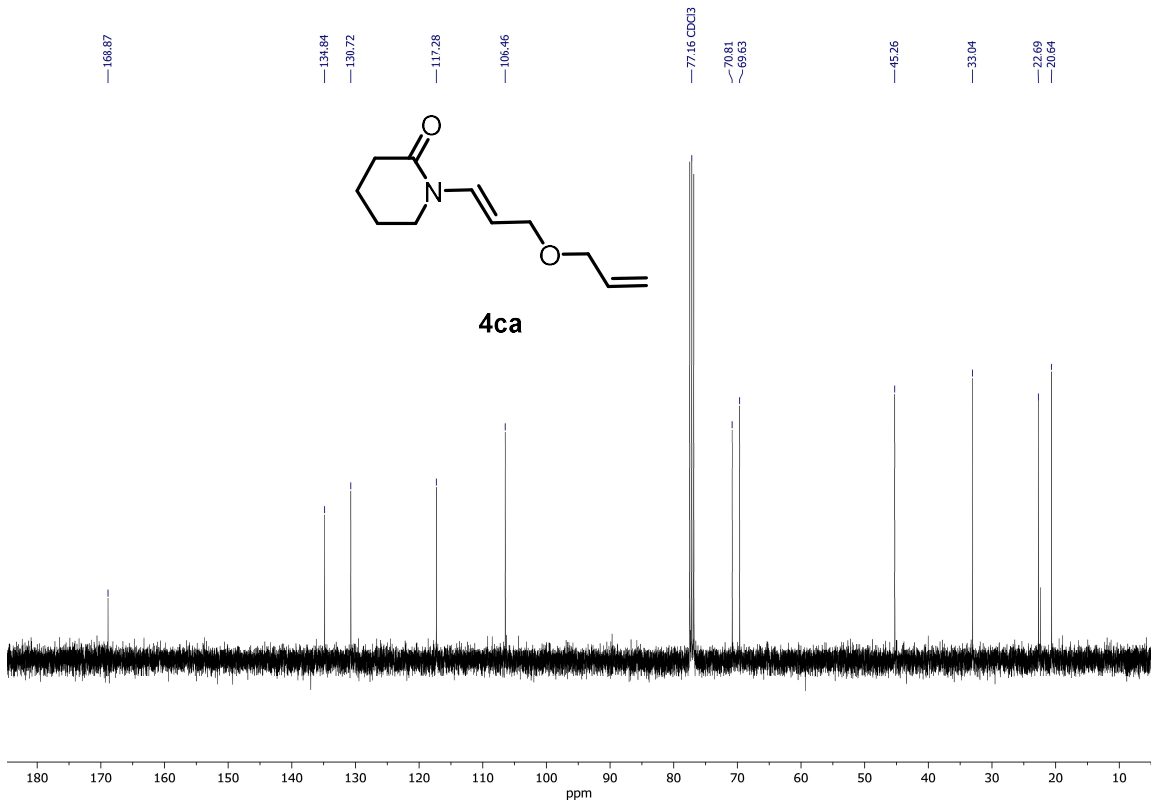
^{1}H-^{13}C HSQC



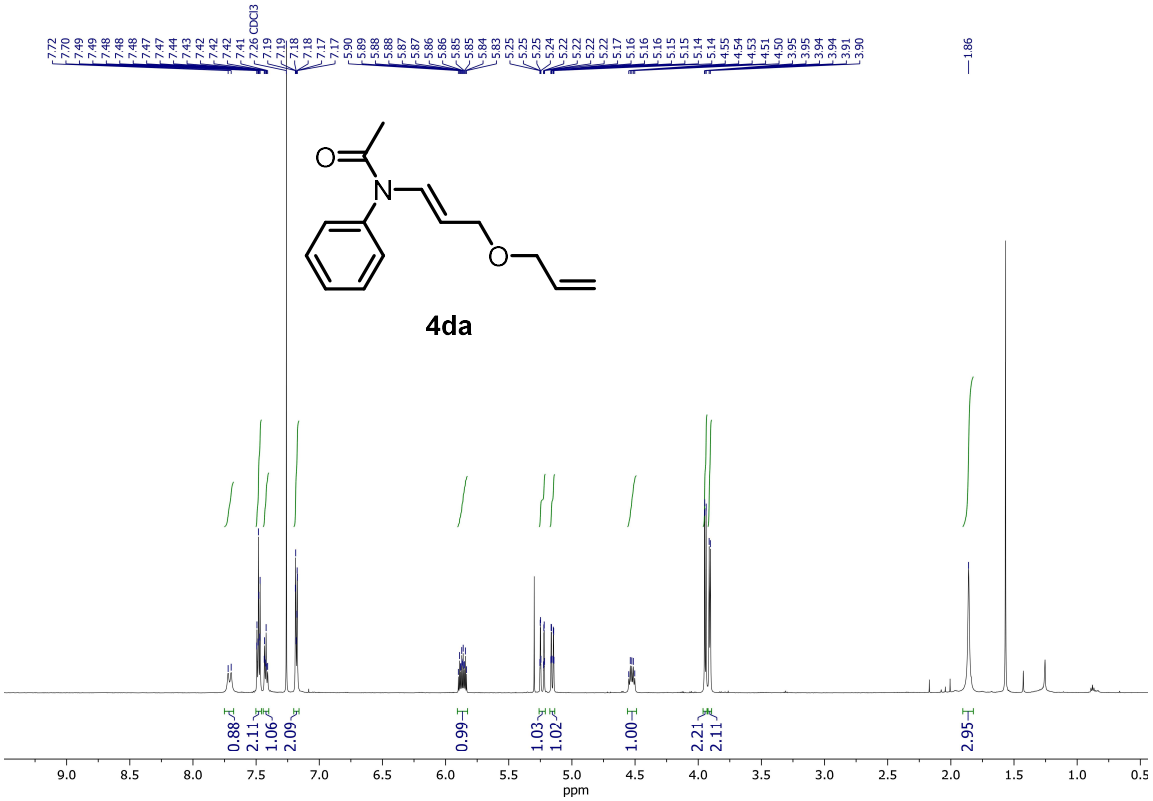
^{1}H NMR (400 MHz, $CDCl_3$)



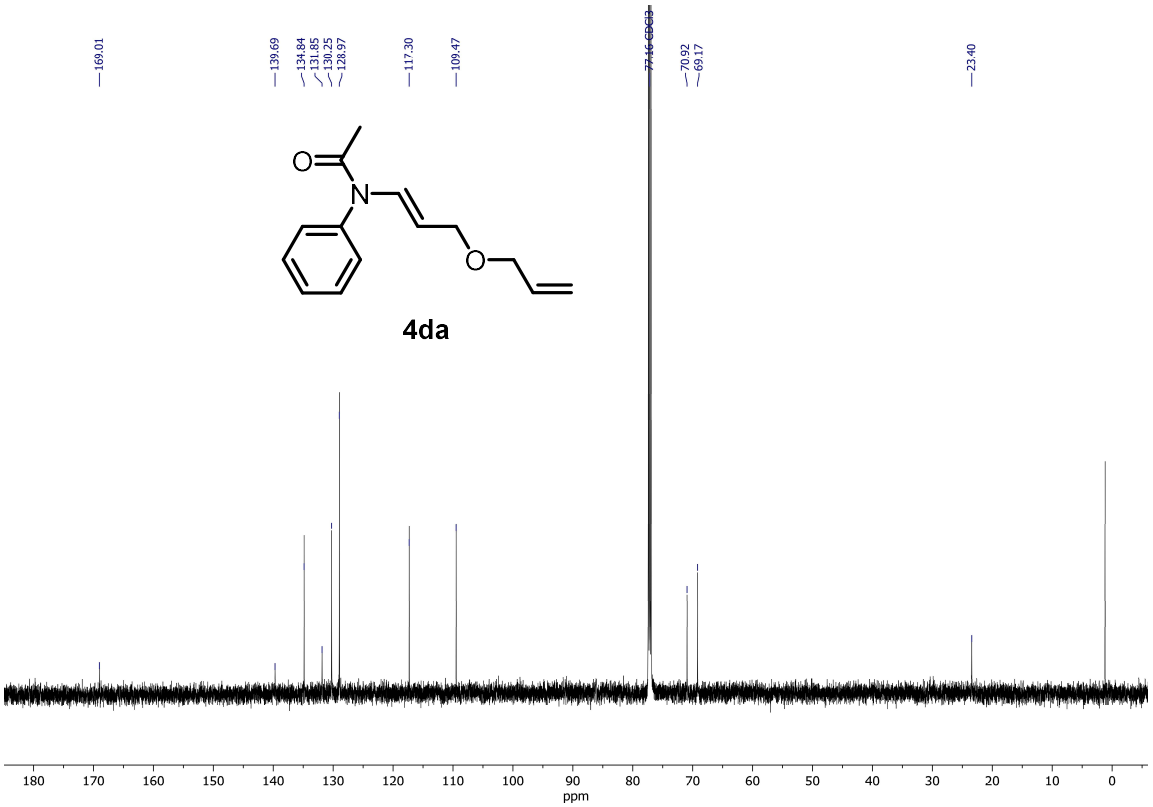
^{13}C NMR (100 MHz, $CDCl_3$)



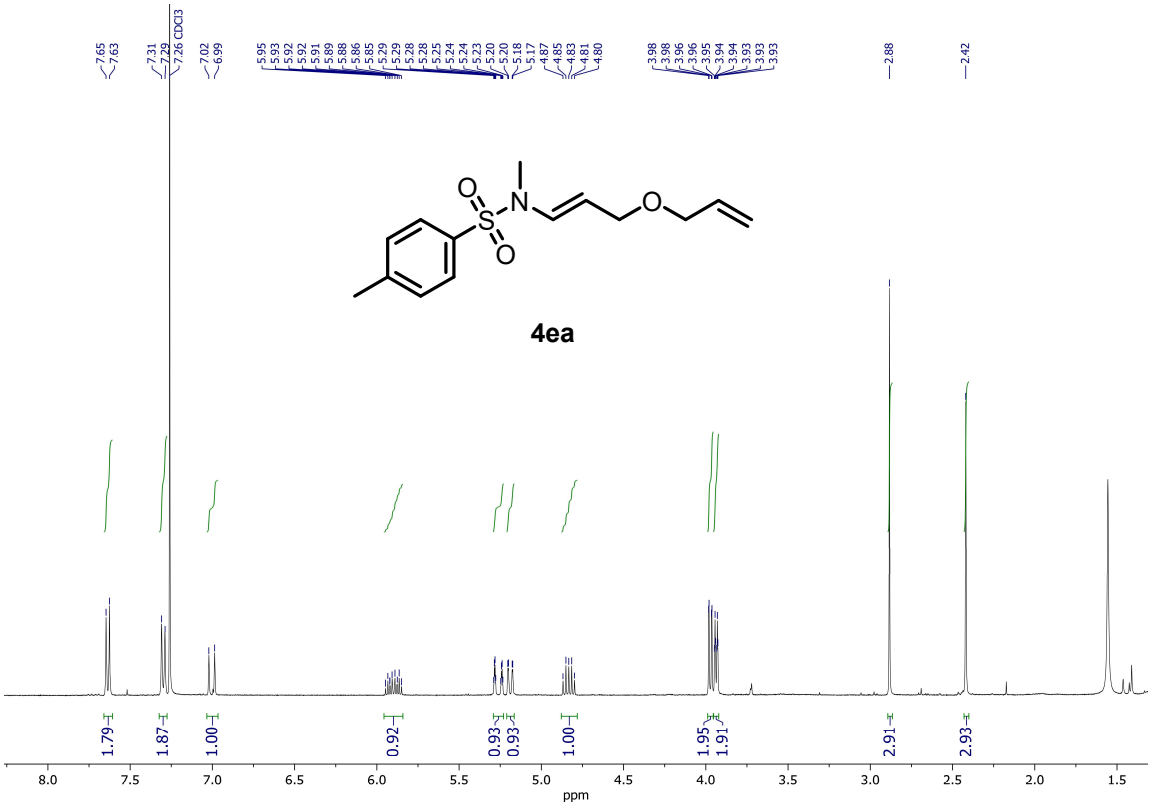
^{1}H NMR (600 MHz, $CDCl_3$)



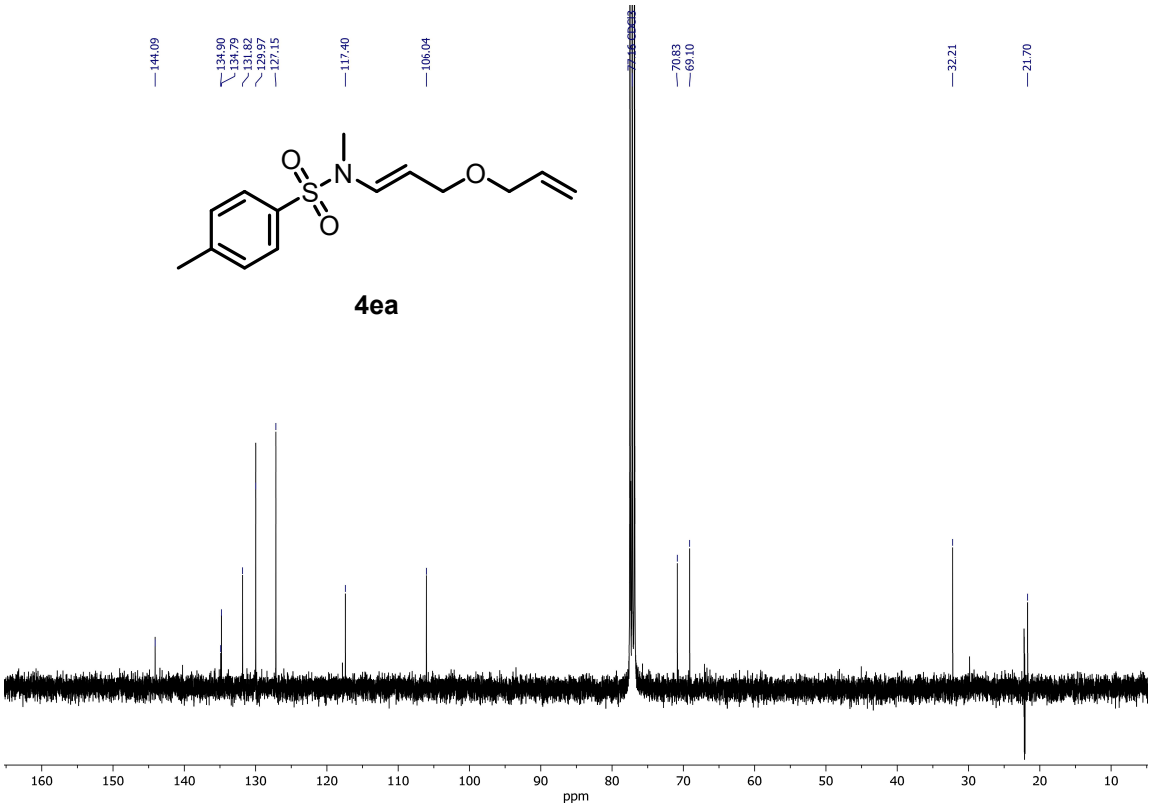
^{13}C NMR (150 MHz, $CDCl_3$)



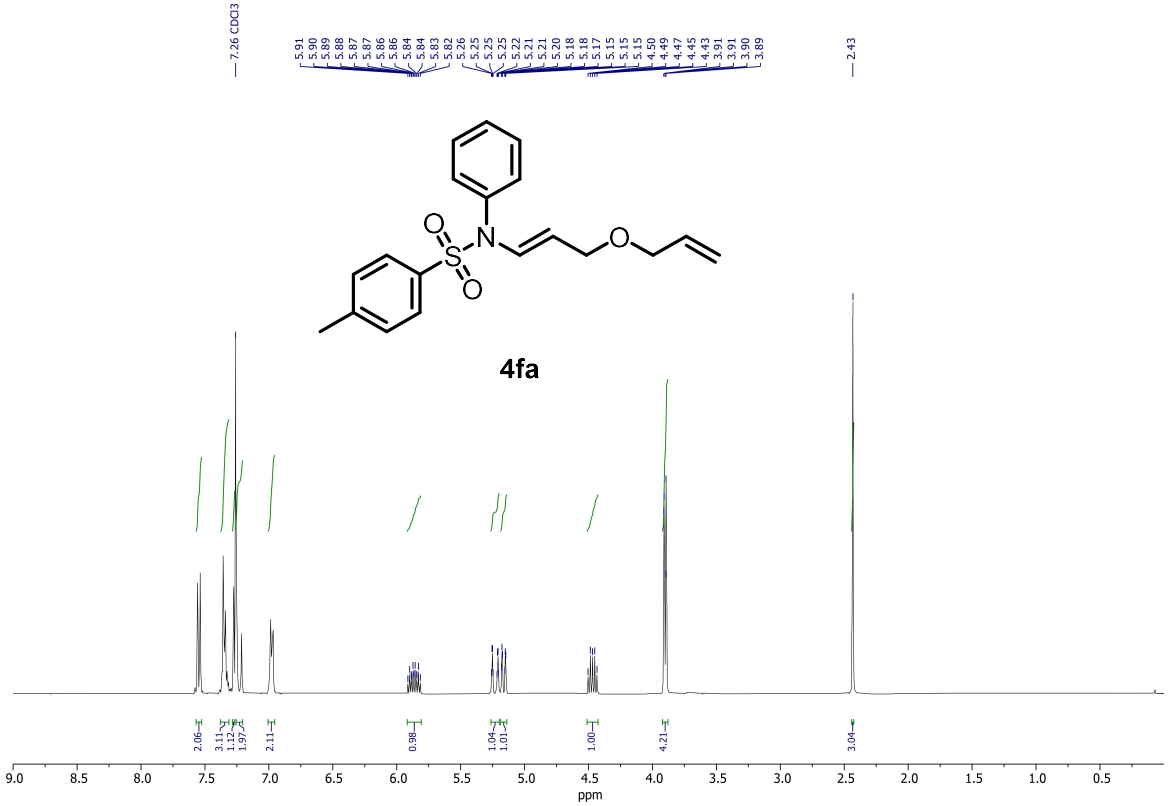
^{1}H NMR (400 MHz, $CDCl_3$)



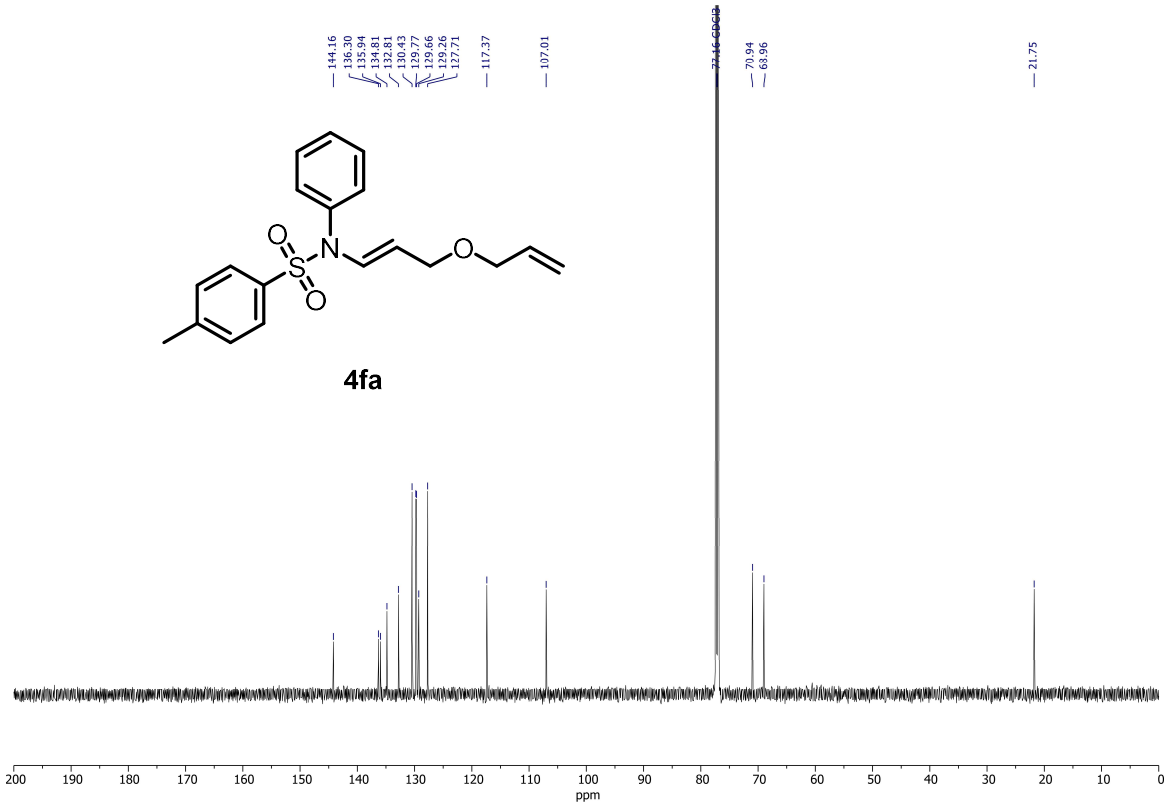
^{13}C NMR (100 MHz, $CDCl_3$)



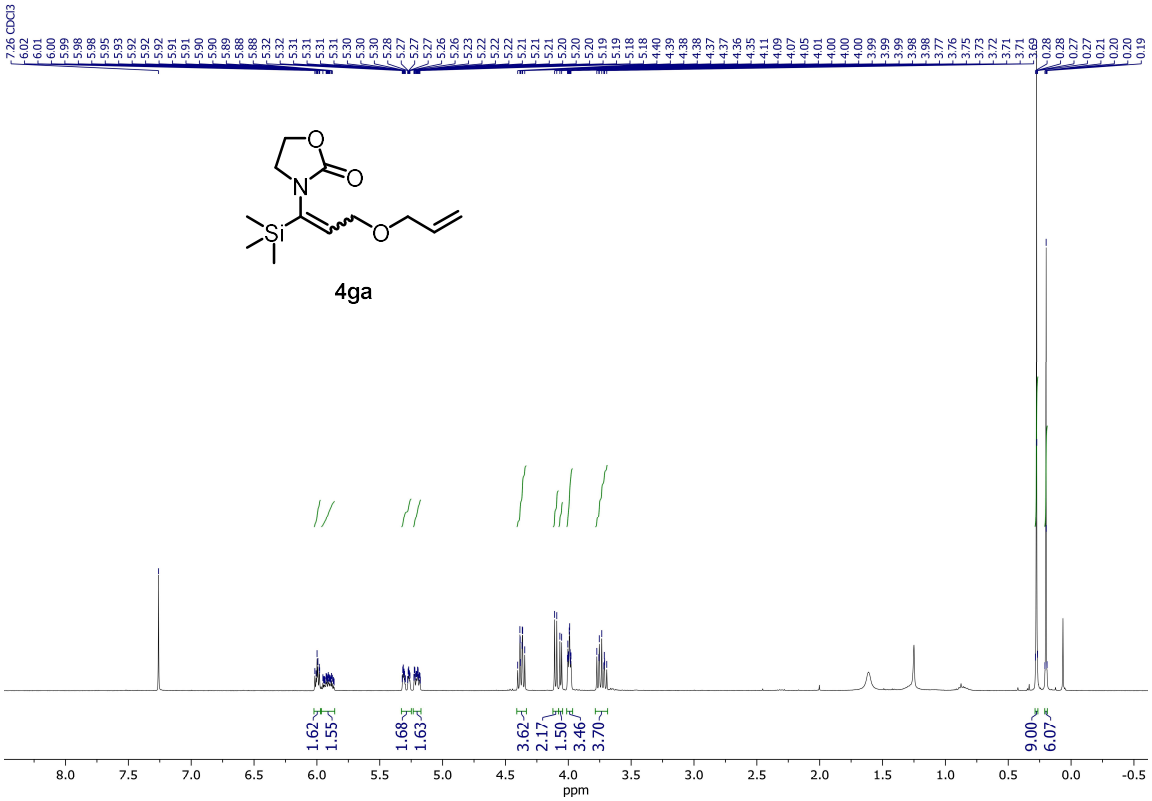
^{1}H NMR (400 MHz, $CDCl_3$)



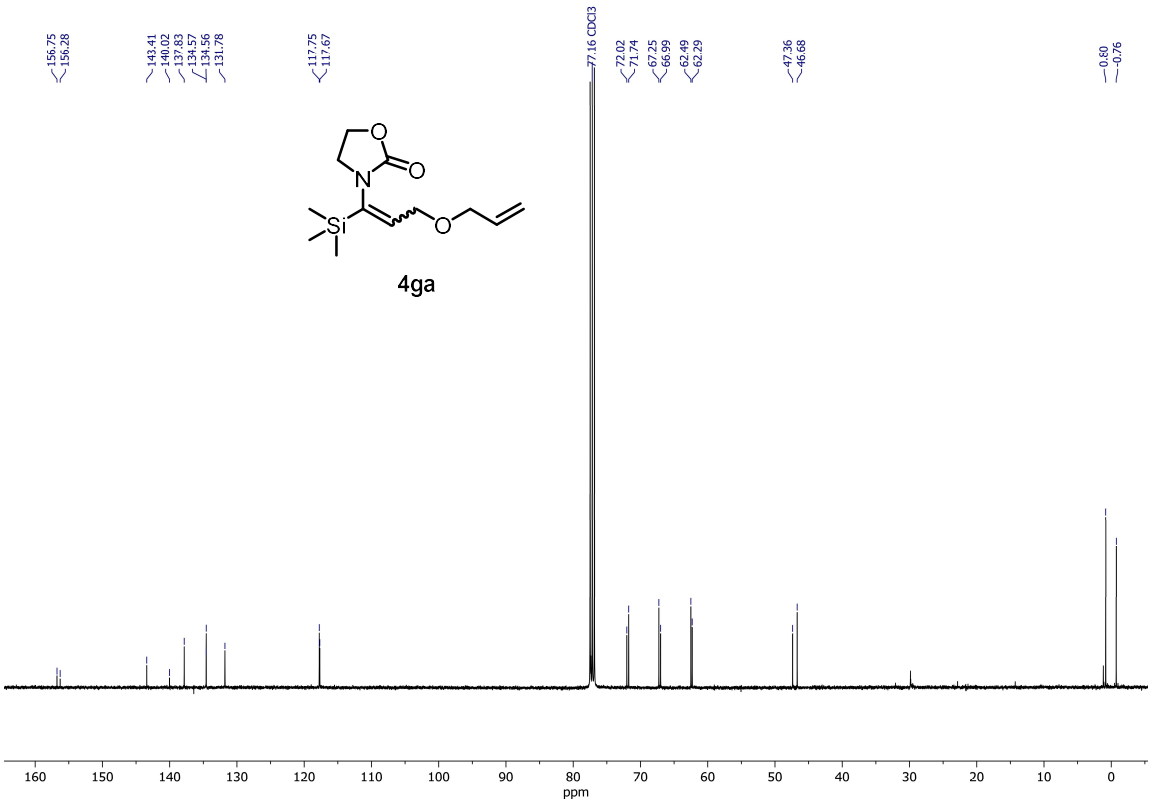
^{13}C NMR (100 MHz, $CDCl_3$)



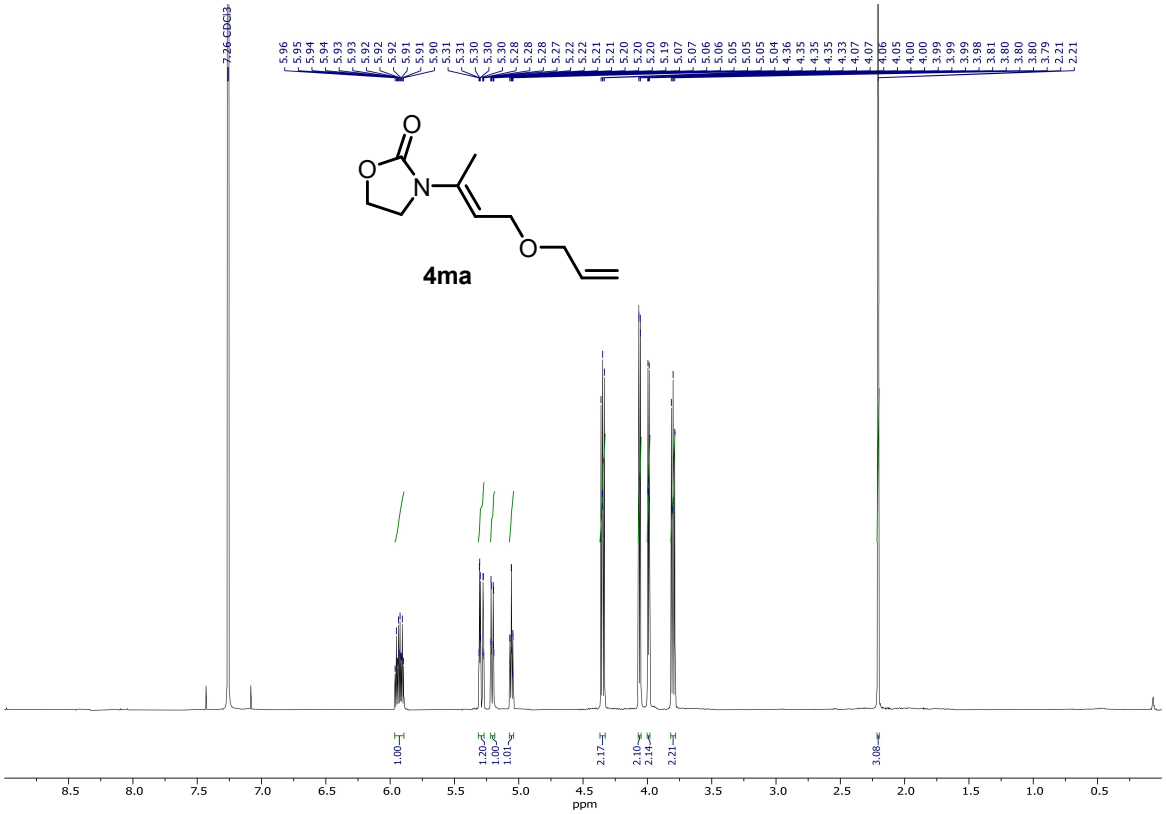
^{1}H NMR (400 MHz, $CDCl_3$)



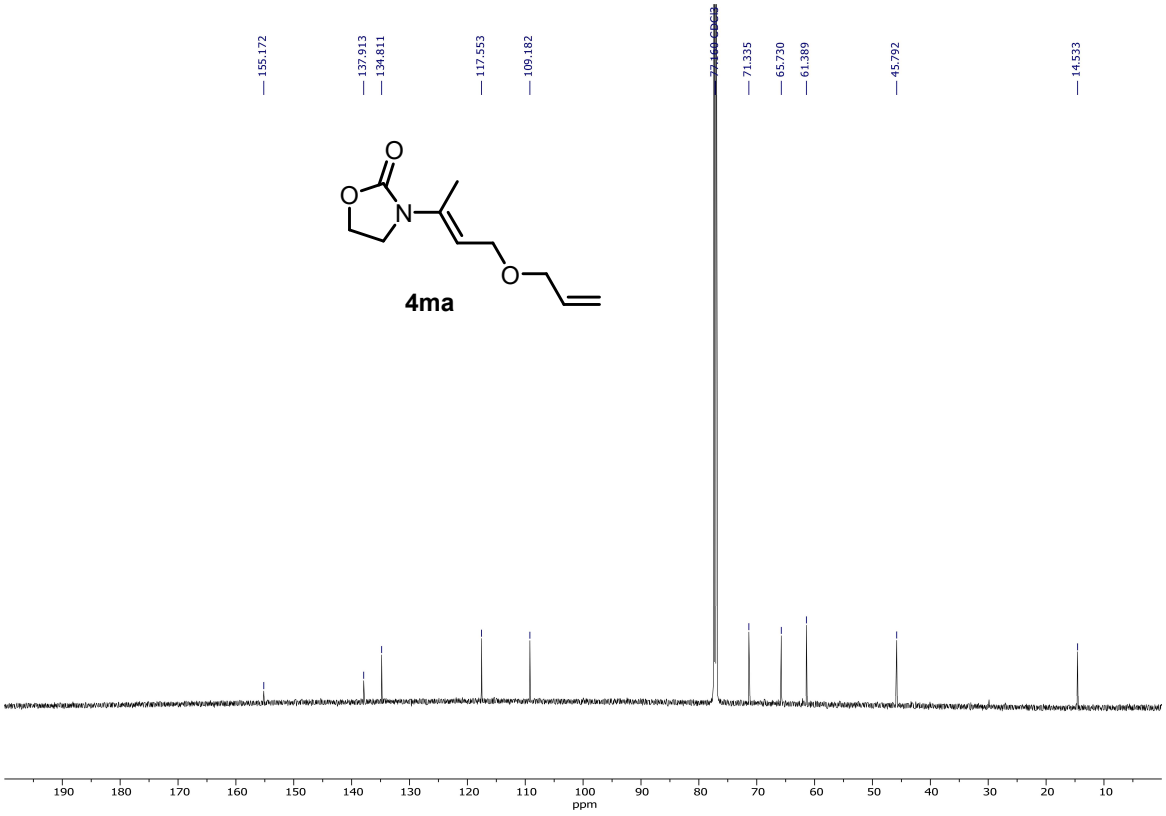
^{13}C NMR (100 MHz, $CDCl_3$)



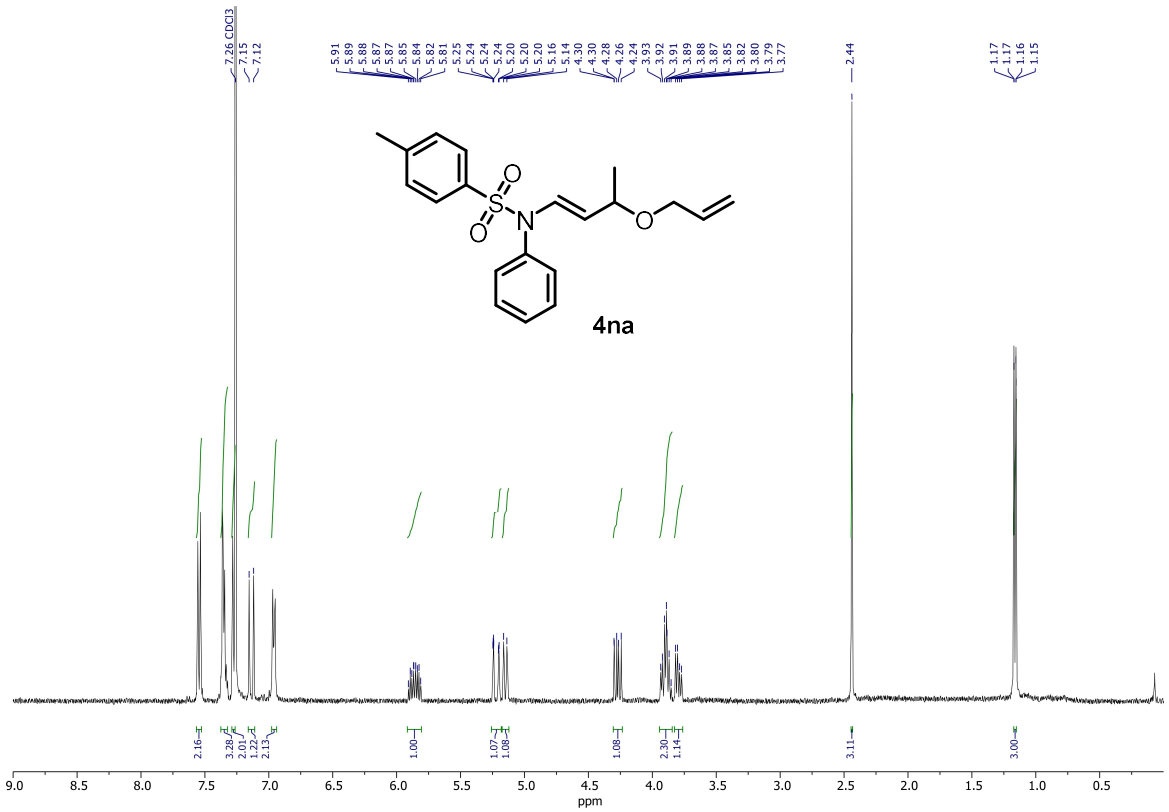
^{1}H NMR (600 MHz, $CDCl_3$)



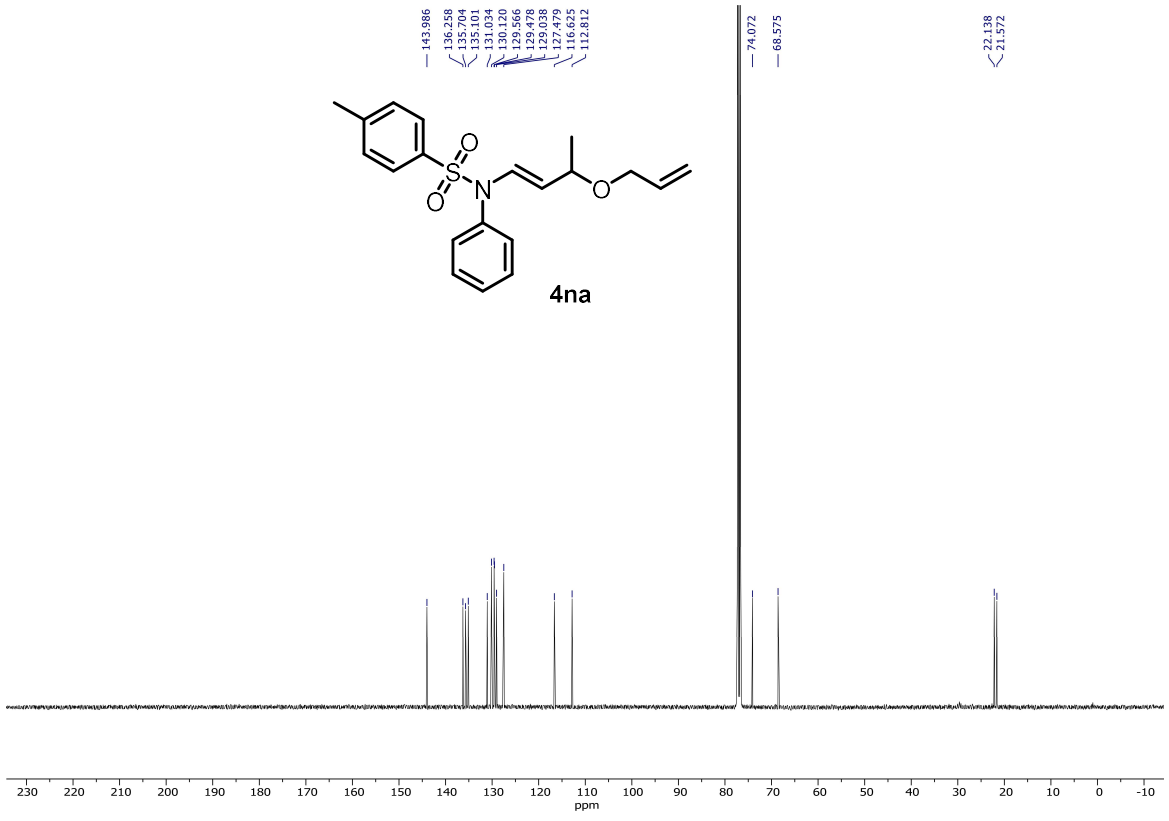
^{13}C NMR (150 MHz, $CDCl_3$)



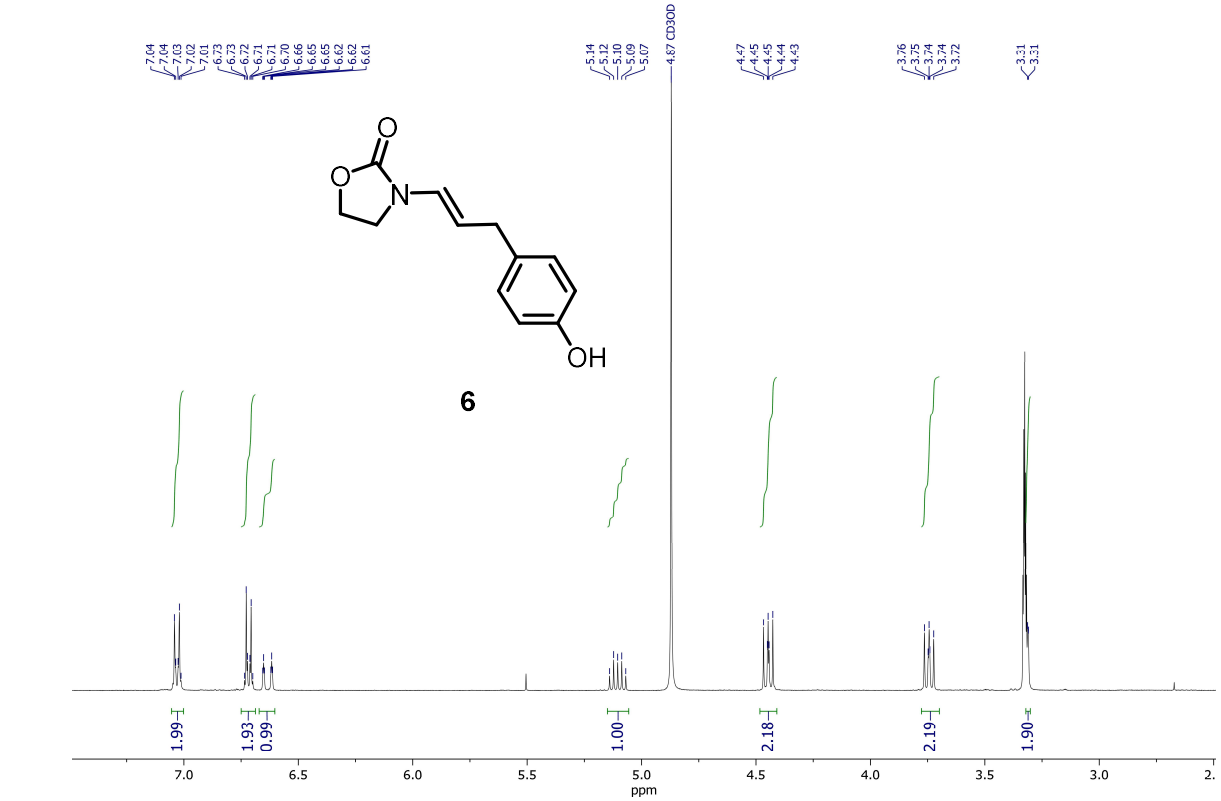
^{1}H NMR (400 MHz, $CDCl_3$)



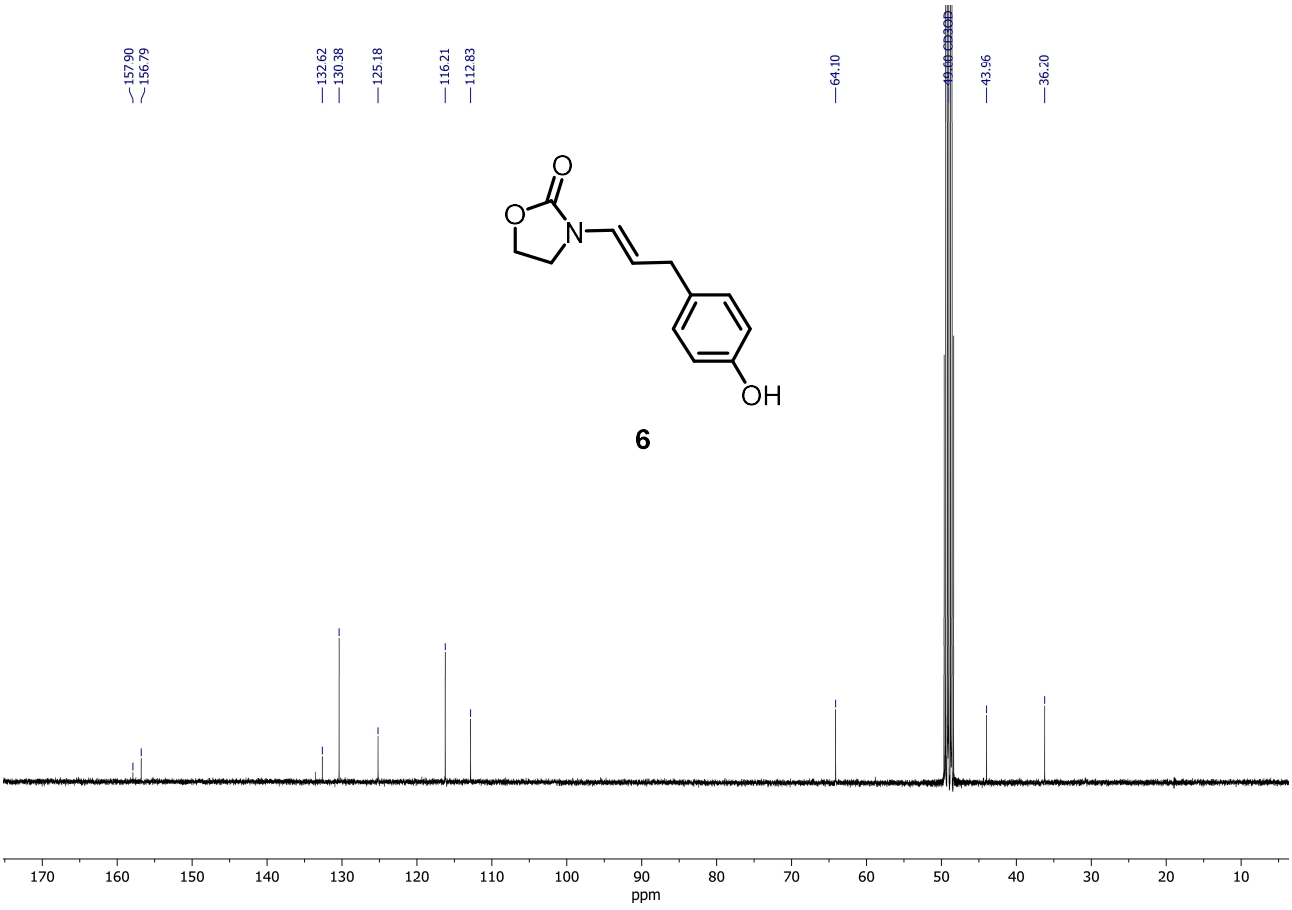
^{13}C NMR (100 MHz, $CDCl_3$)



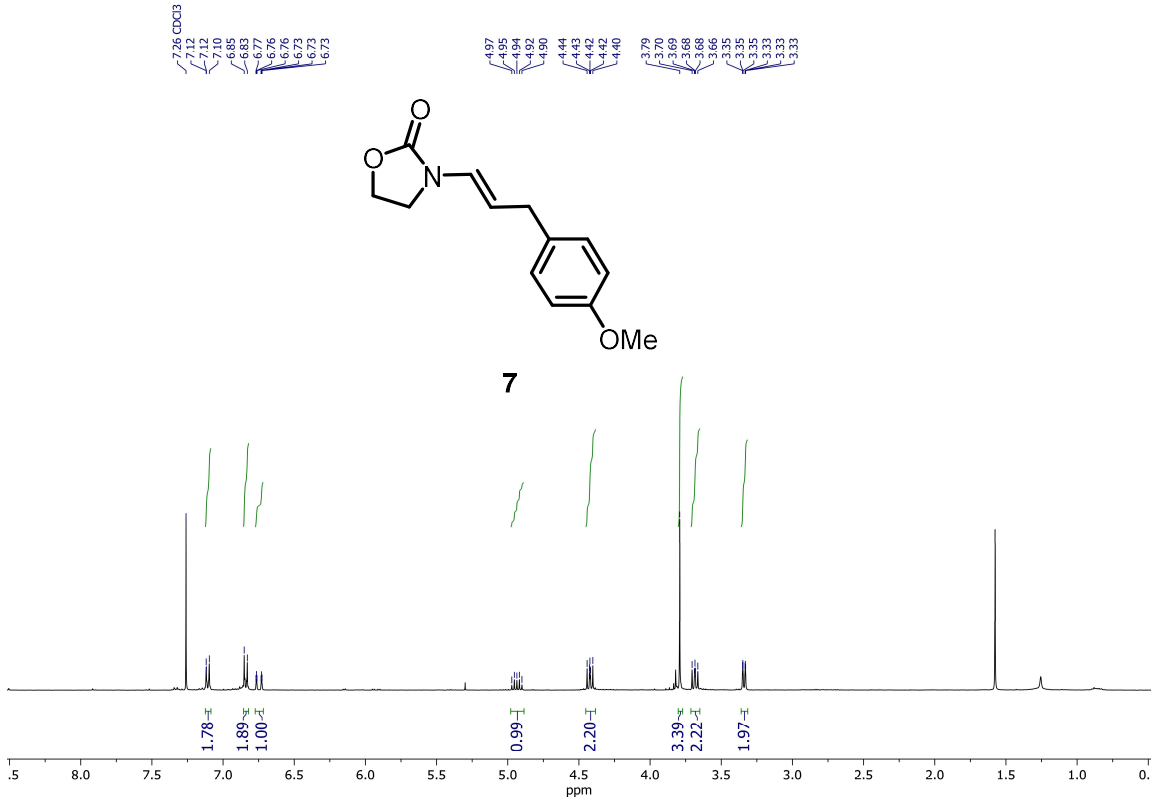
^{1}H NMR (400 MHz, CD_3OD)



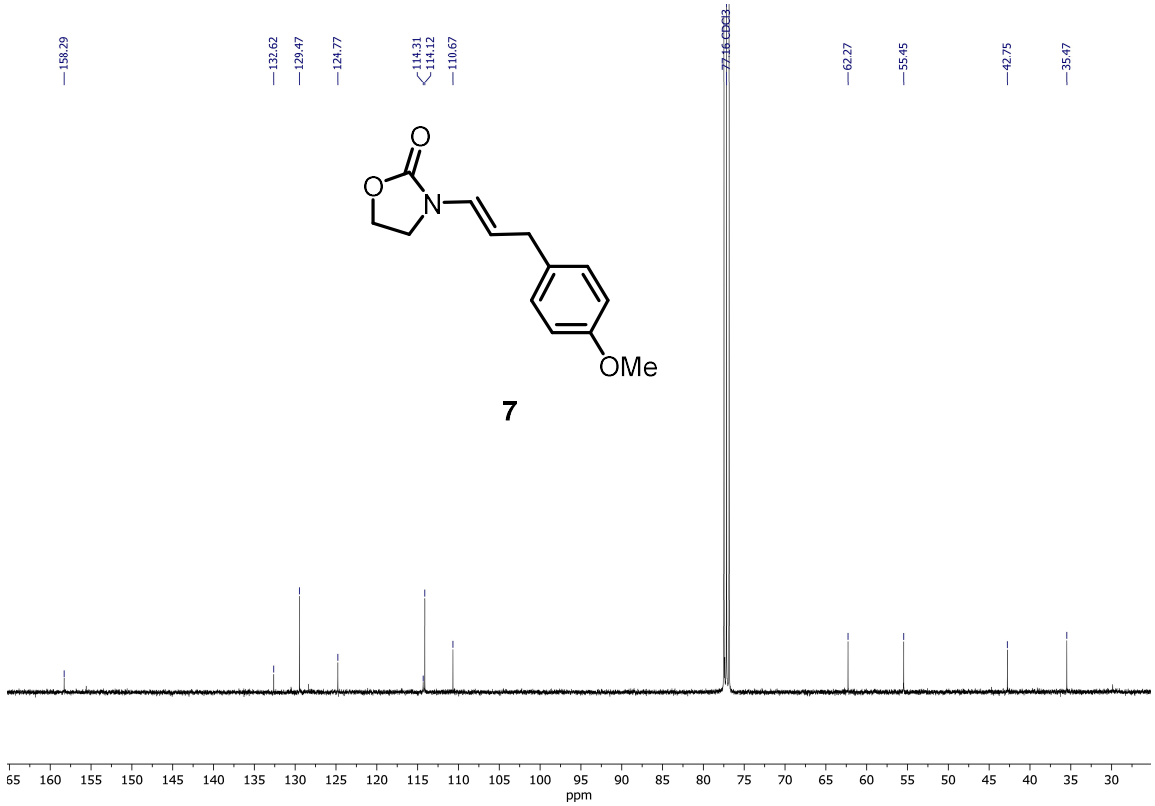
^{13}C NMR (100 MHz, CD_3OD)



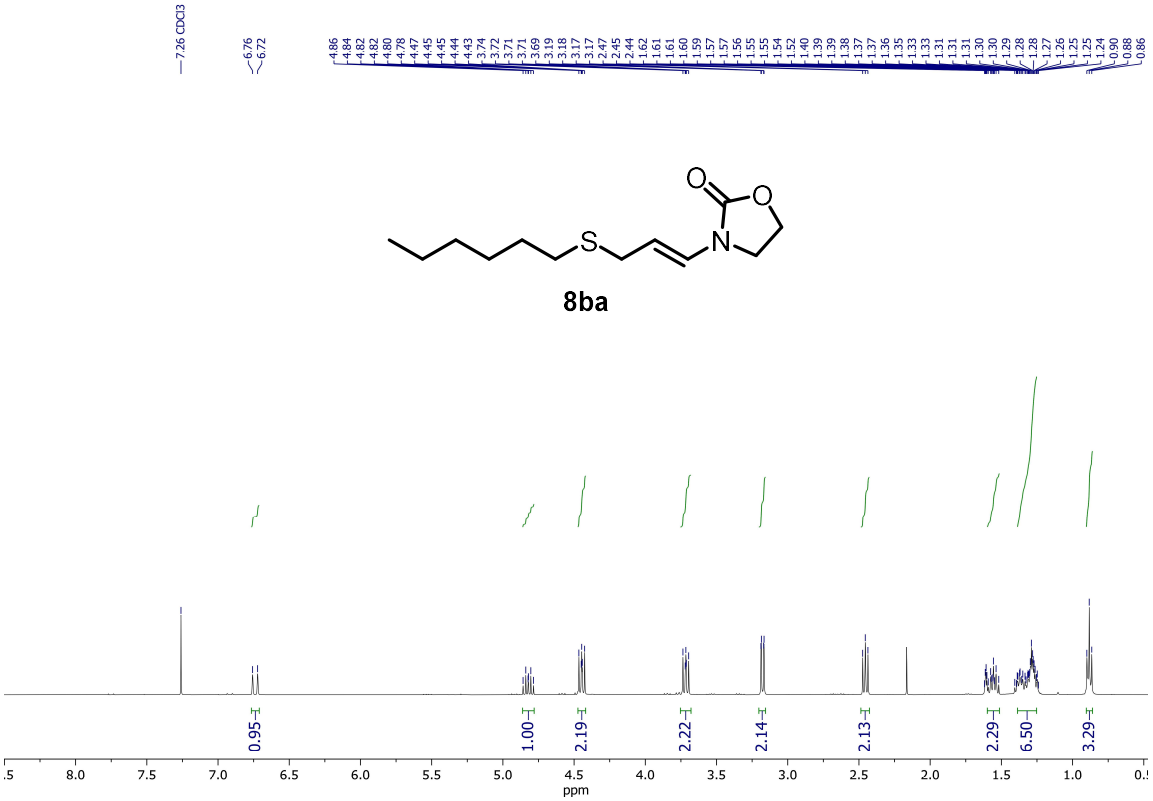
^{1}H NMR (400 MHz, $CDCl_3$)



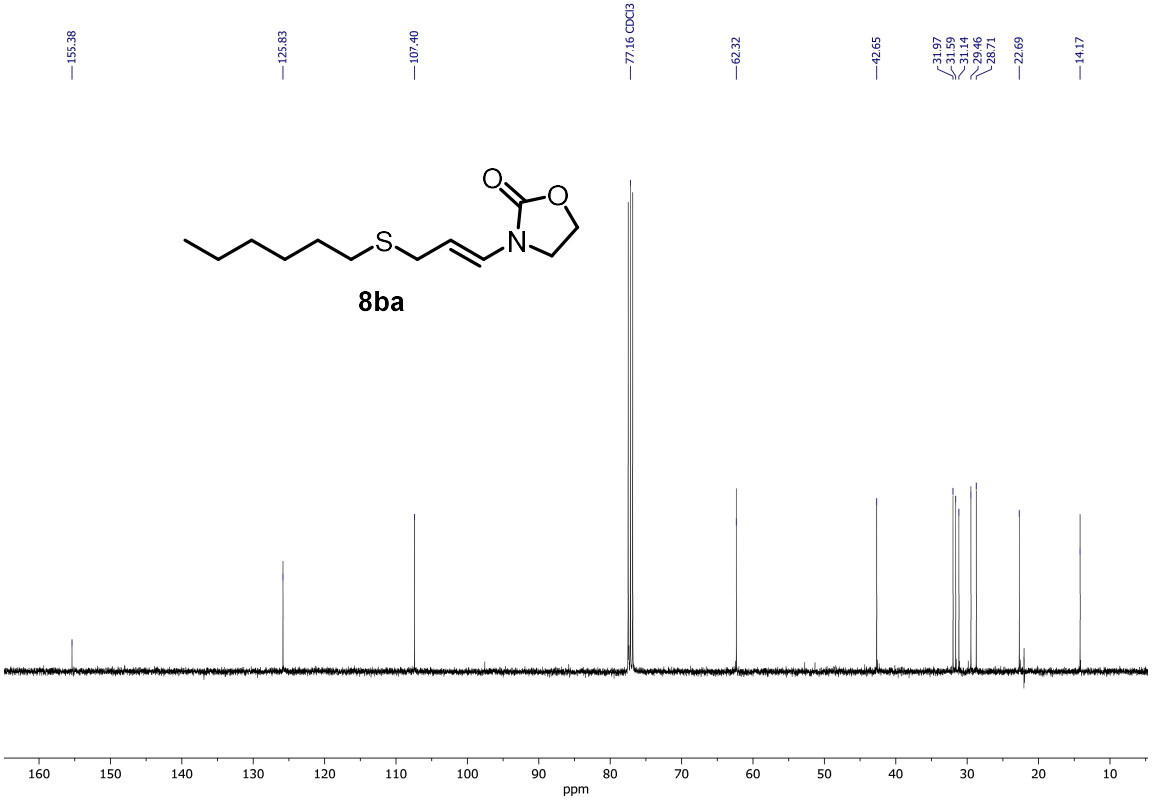
^{13}C NMR (100 MHz, $CDCl_3$)



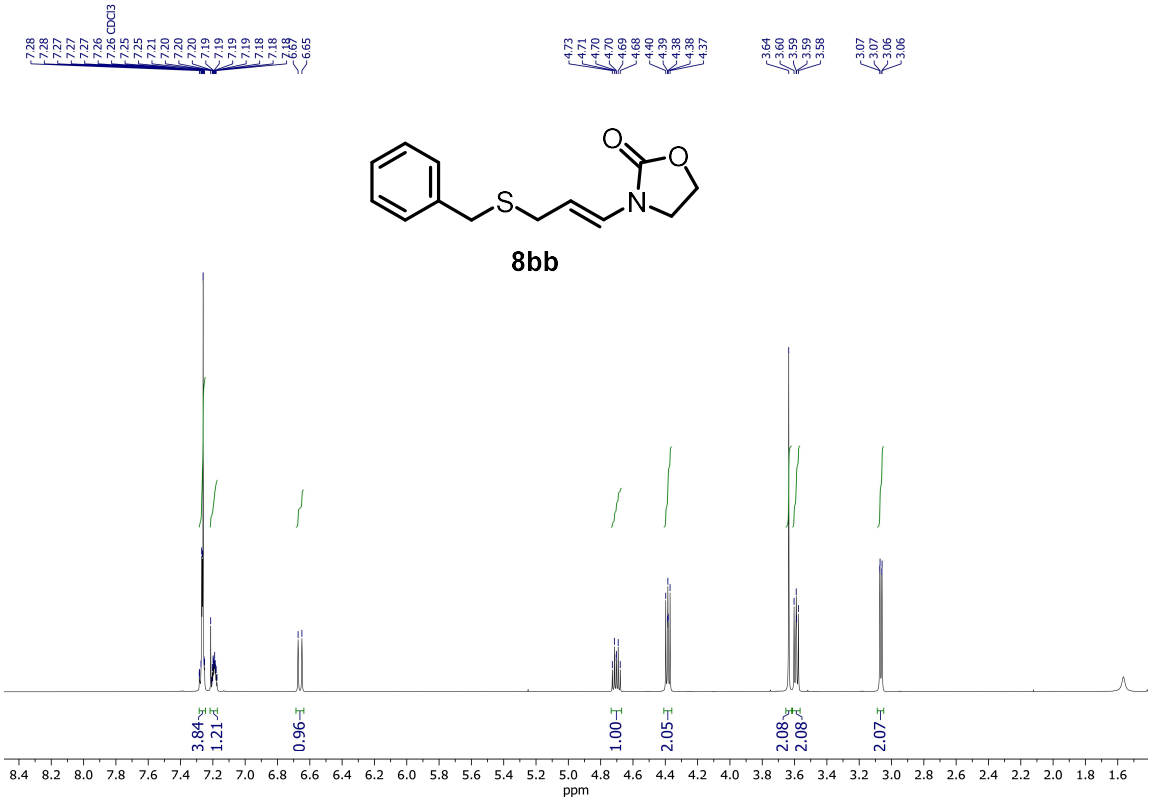
^{1}H NMR (400 MHz, $CDCl_3$)



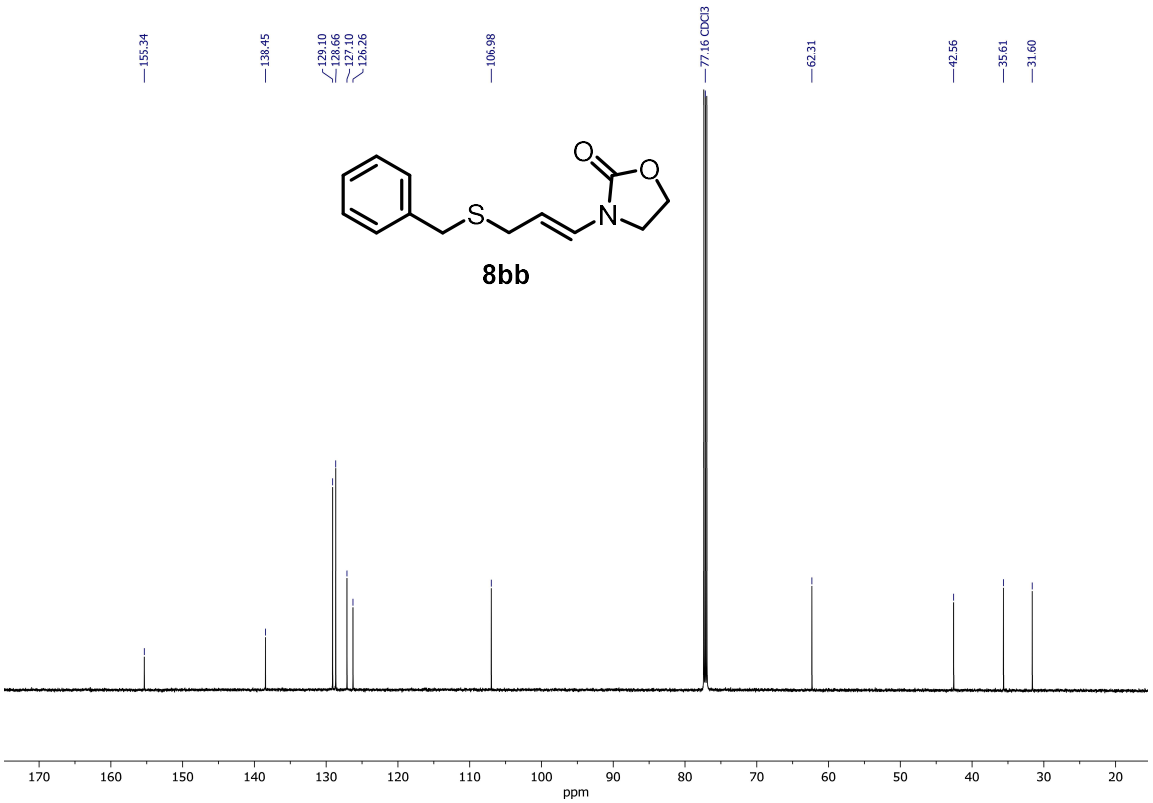
^{13}C NMR (100 MHz, $CDCl_3$)



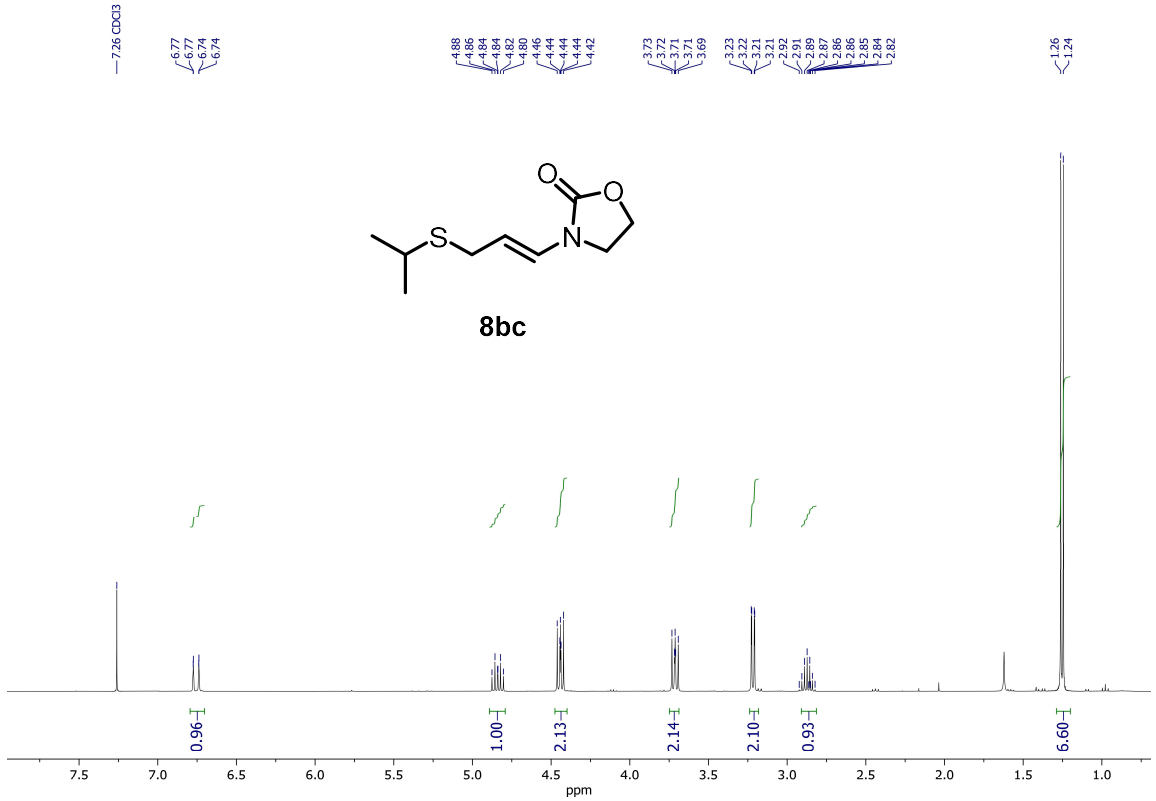
^{1}H NMR (600 MHz, $CDCl_3$)



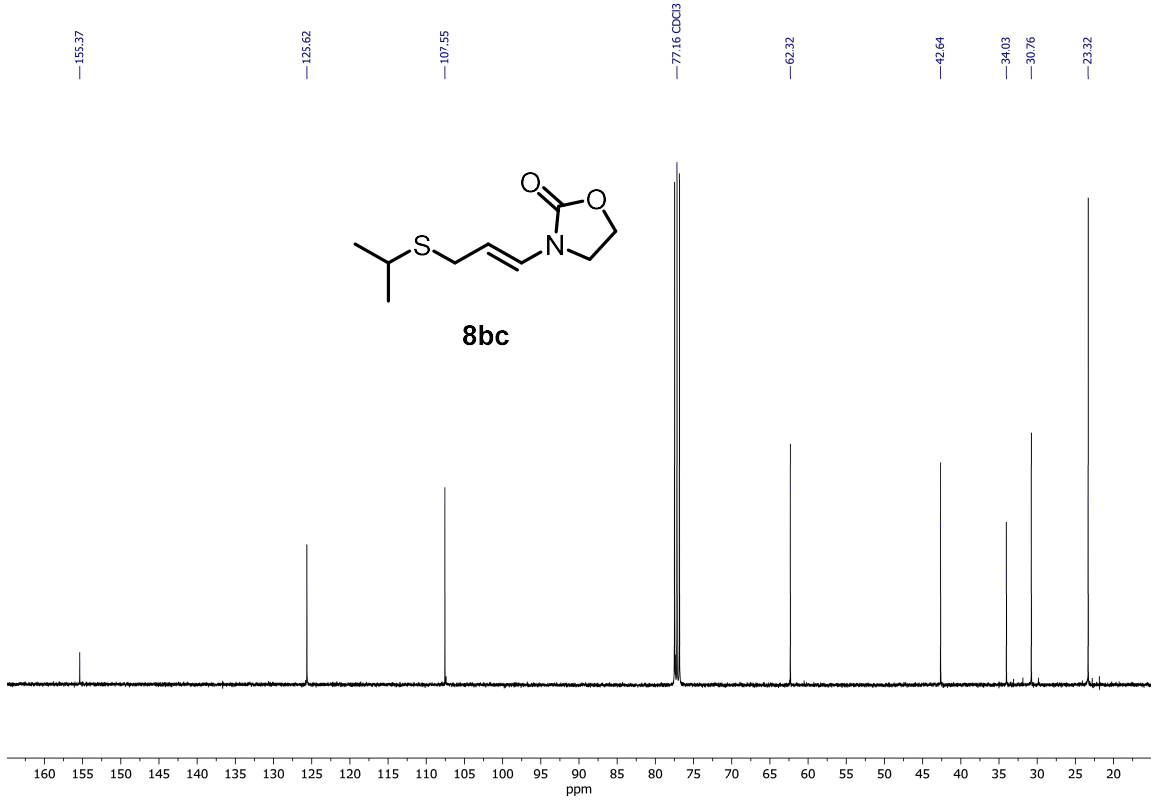
^{13}C NMR (150 MHz, $CDCl_3$)



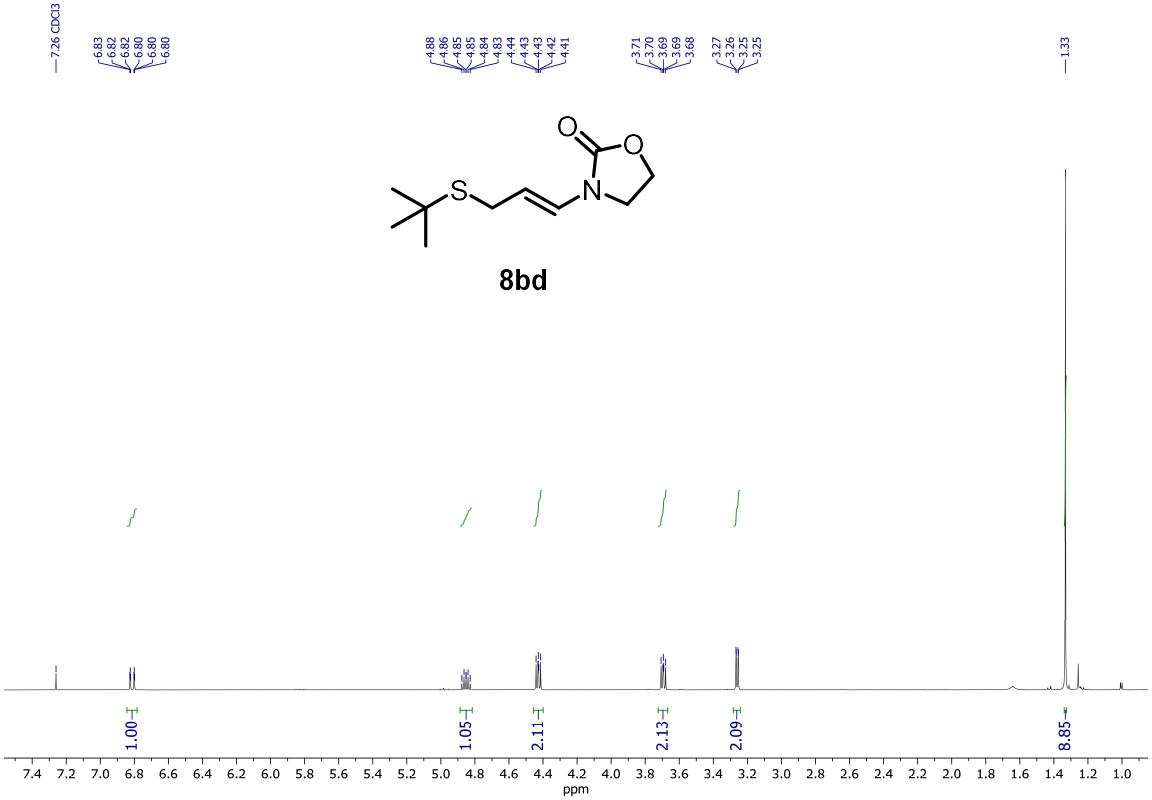
^{1}H NMR (400 MHz, $CDCl_3$)



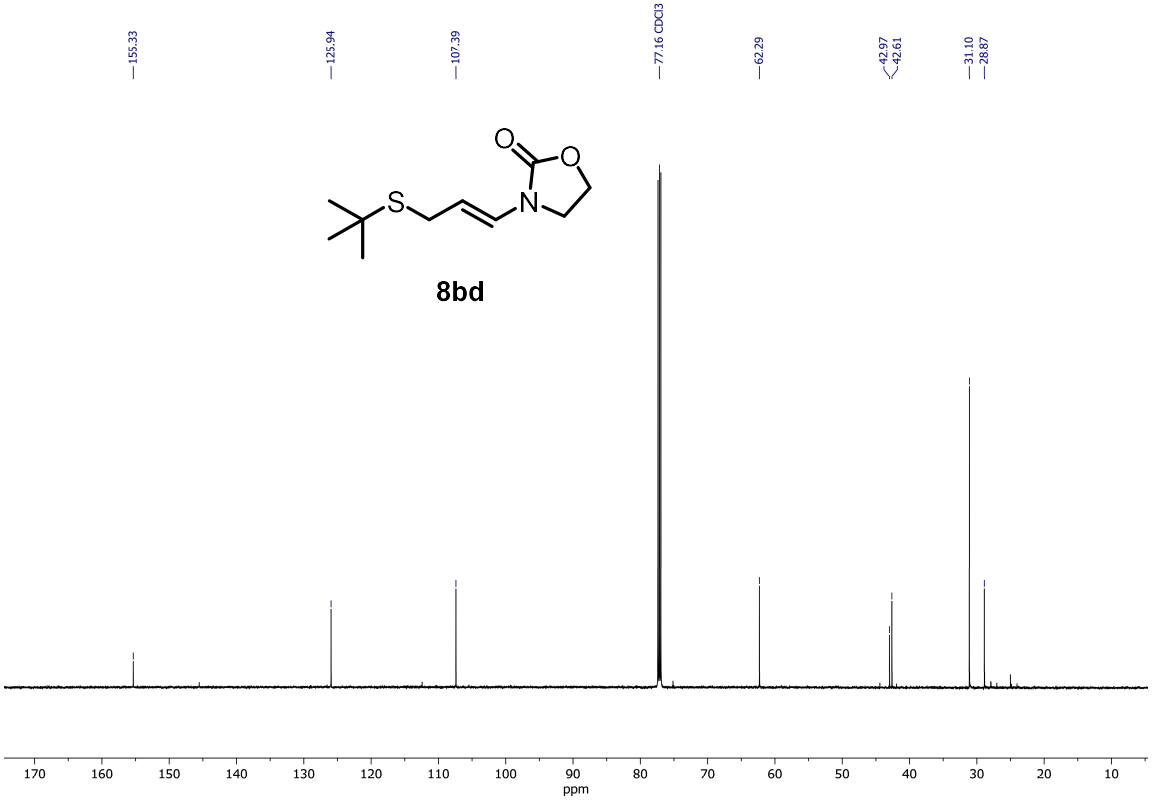
^{13}C NMR (100 MHz, $CDCl_3$)



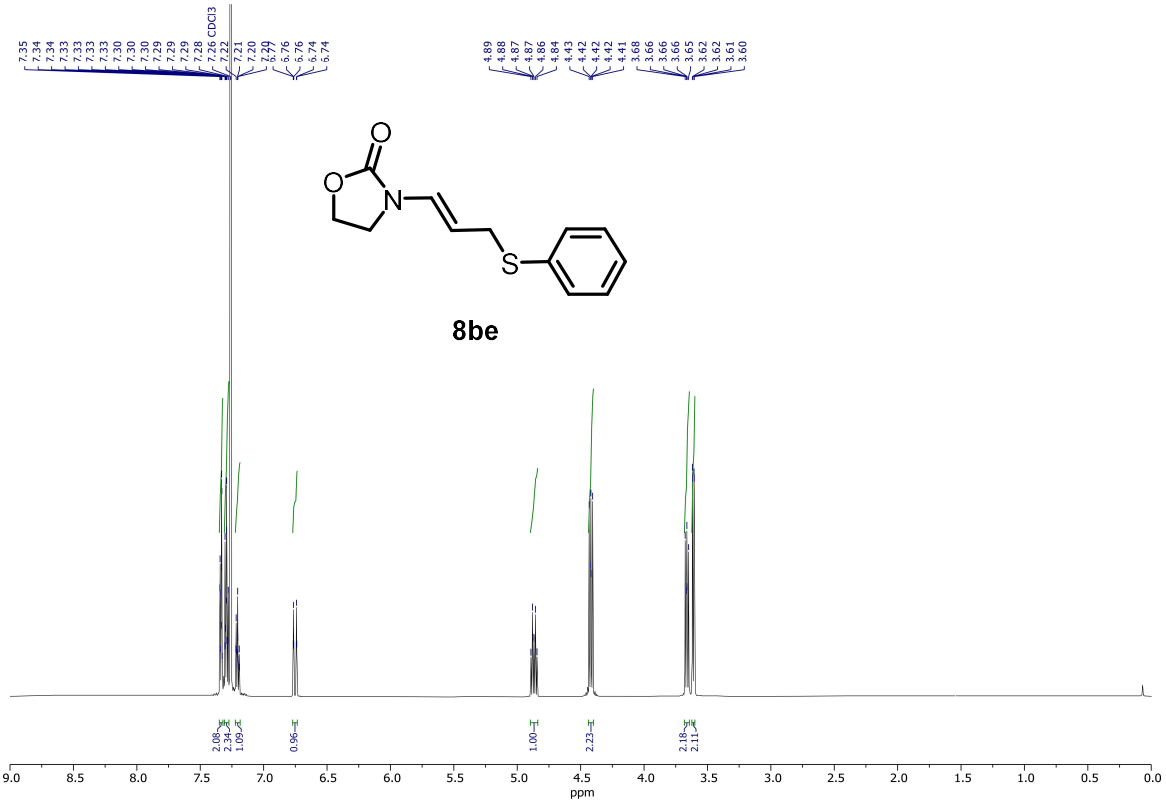
^{1}H NMR (600 MHz, $CDCl_3$)



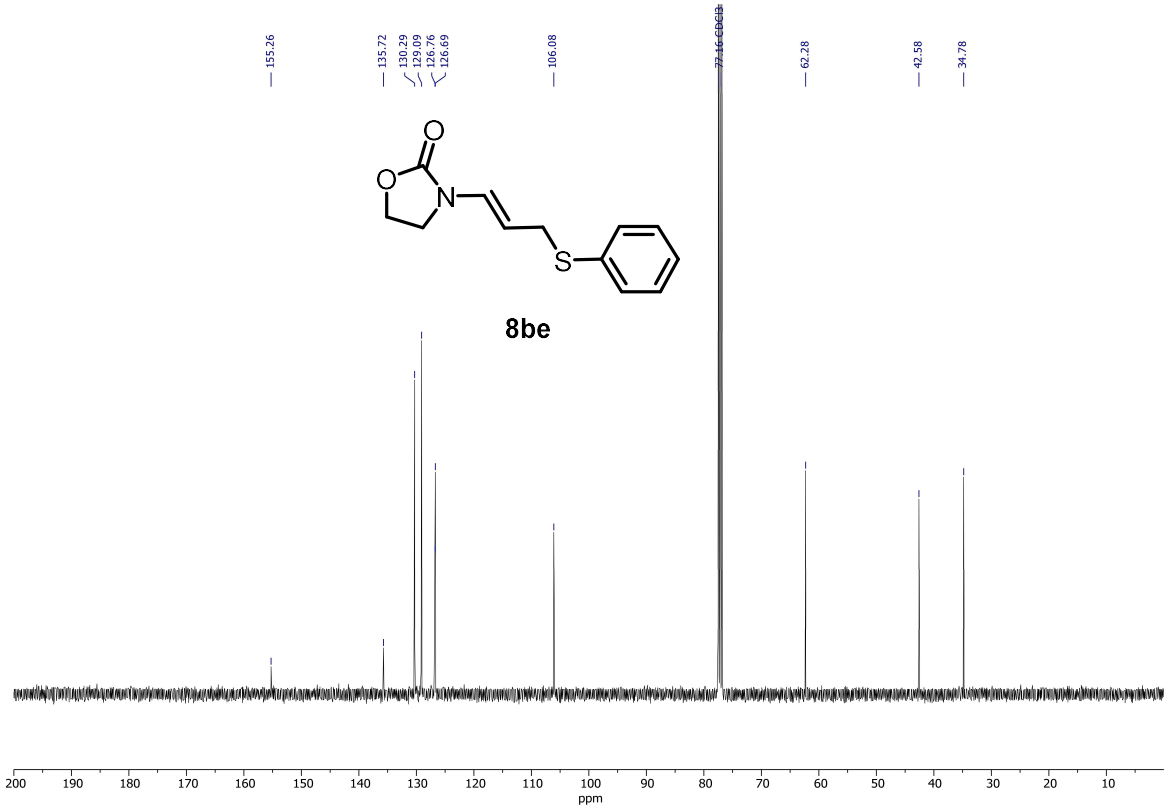
^{13}C NMR (150 MHz, $CDCl_3$)



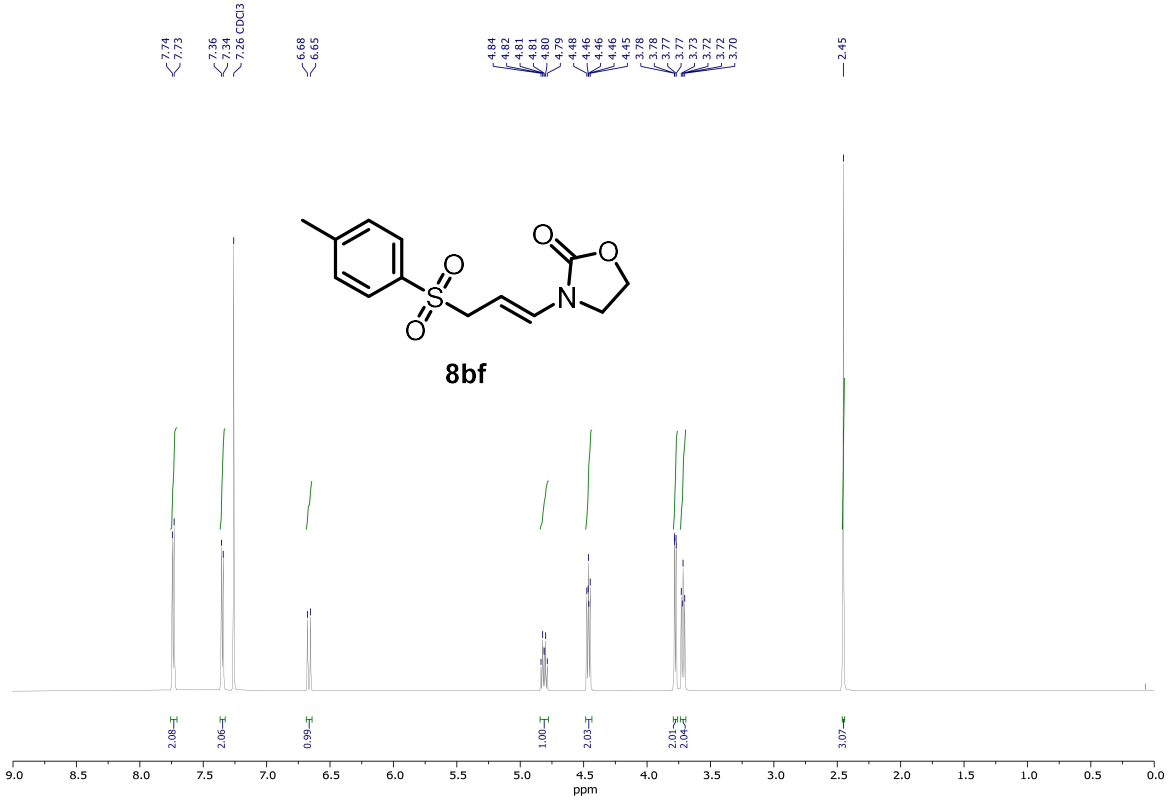
^{1}H NMR (600 MHz, $CDCl_3$)



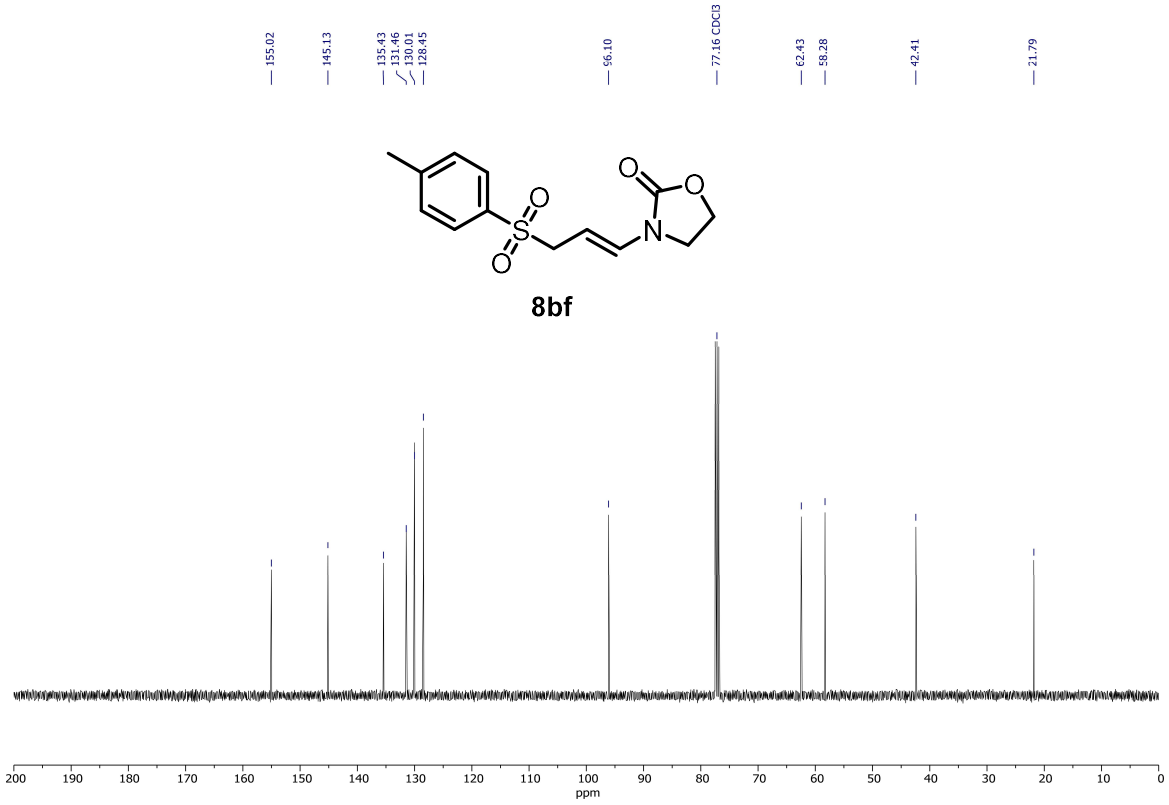
^{13}C NMR (100 MHz, $CDCl_3$)



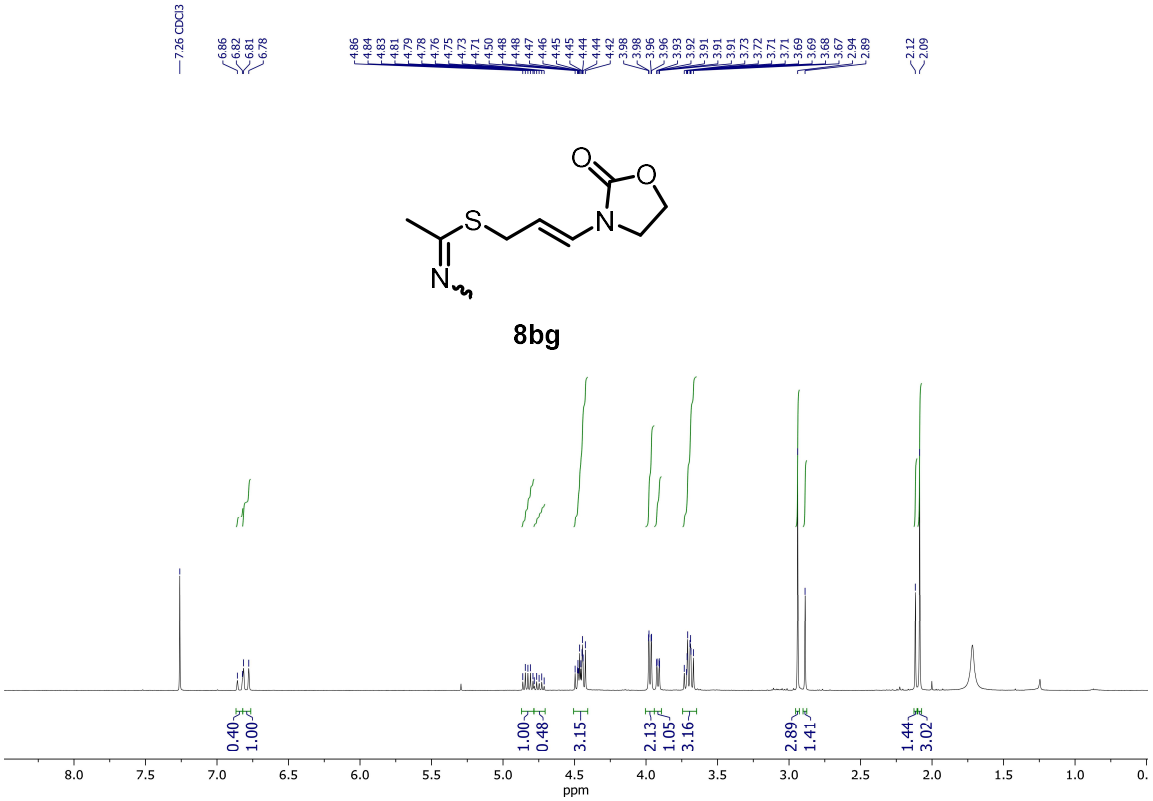
^{1}H NMR (400 MHz, $CDCl_3$)



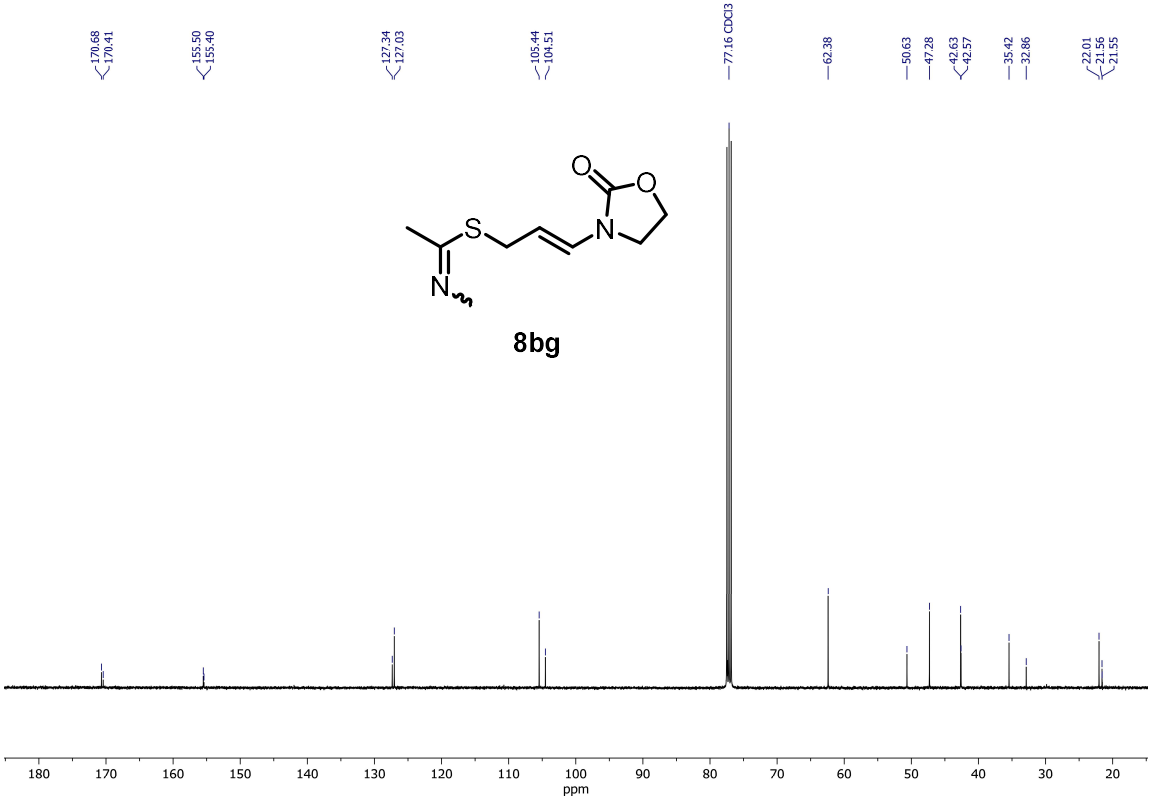
^{13}C NMR (100 MHz, $CDCl_3$)



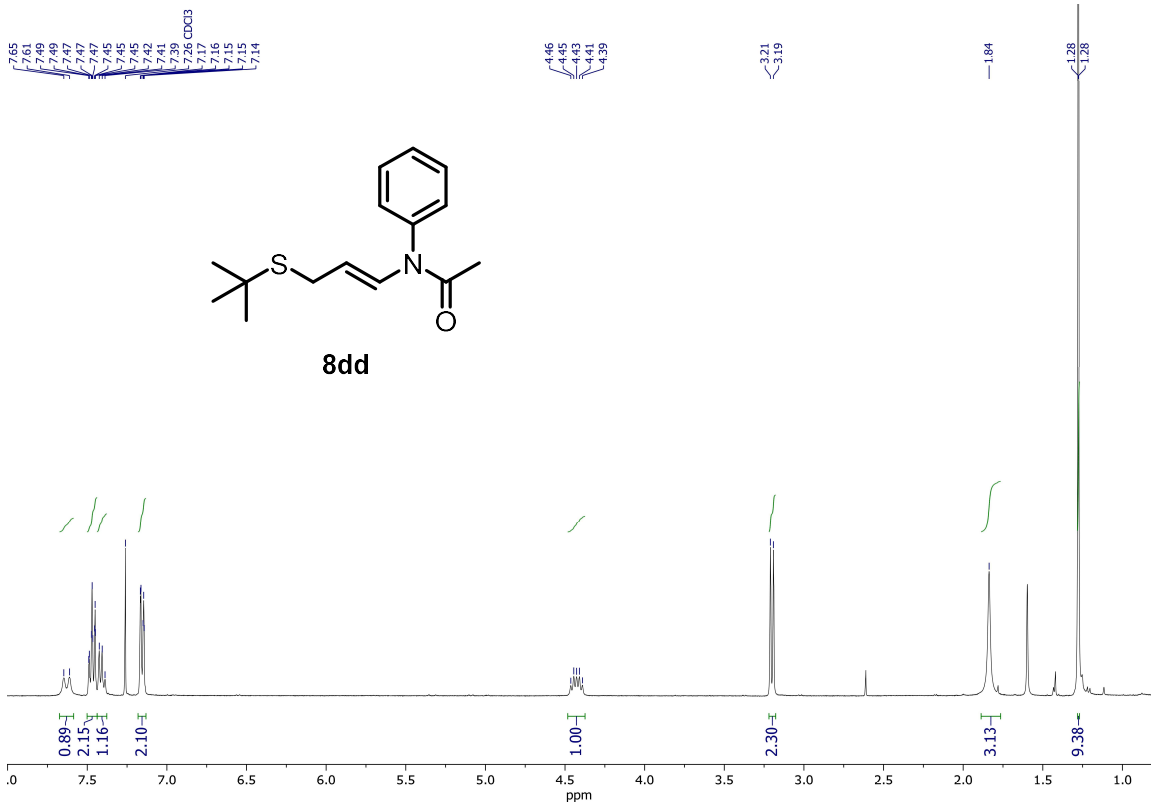
^{1}H NMR (400 MHz, $CDCl_3$)



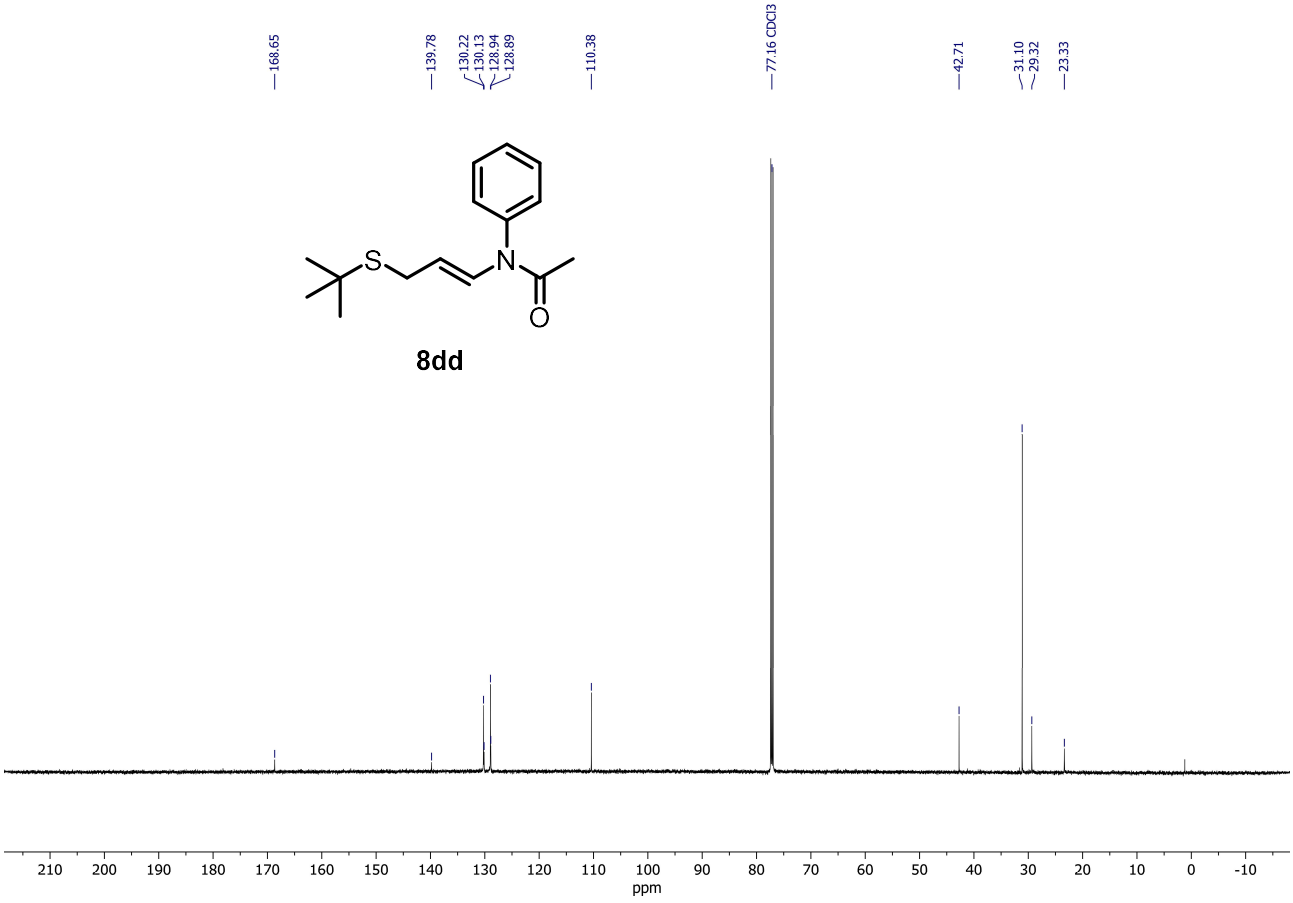
^{13}C NMR (100 MHz, $CDCl_3$)



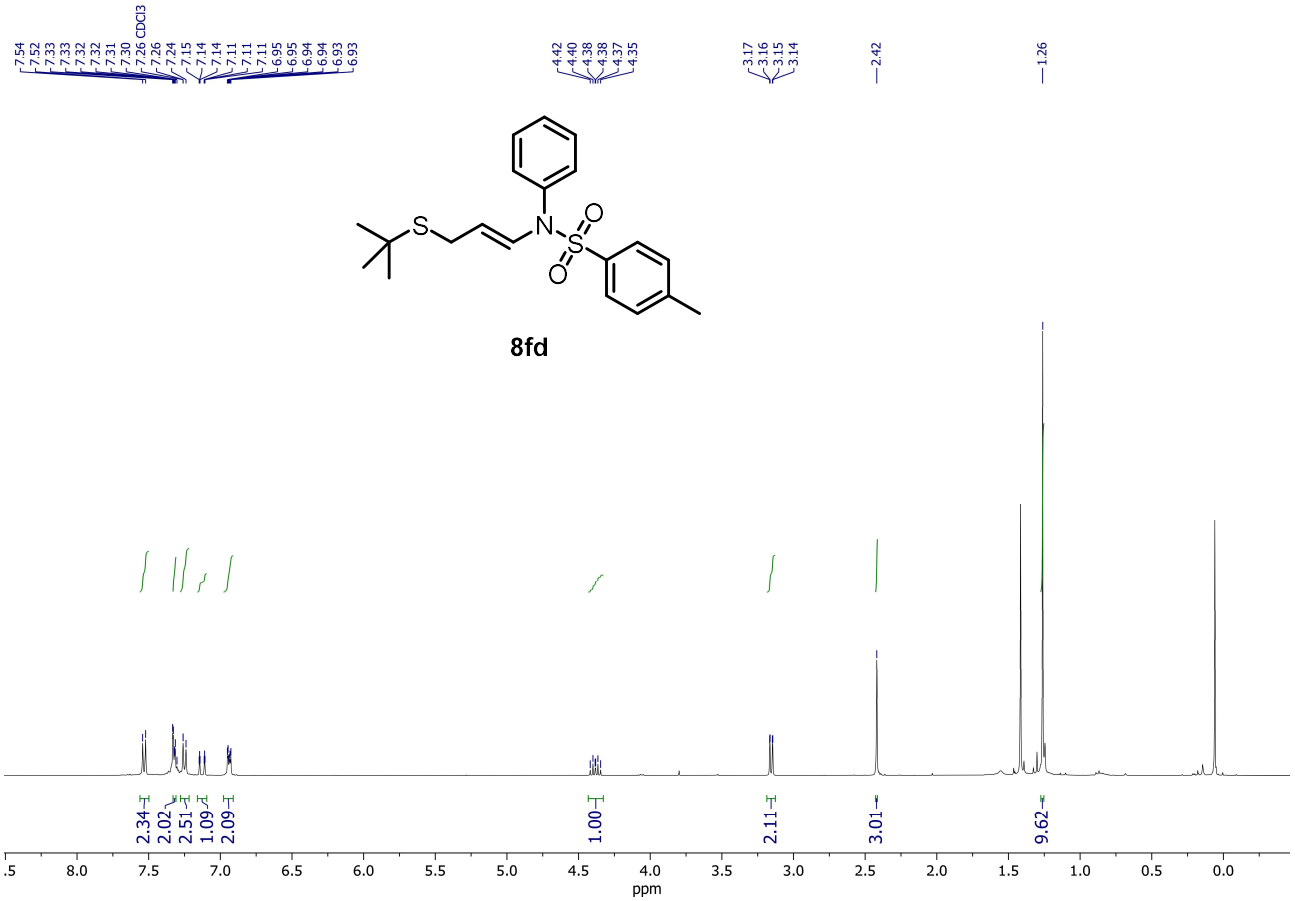
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (150 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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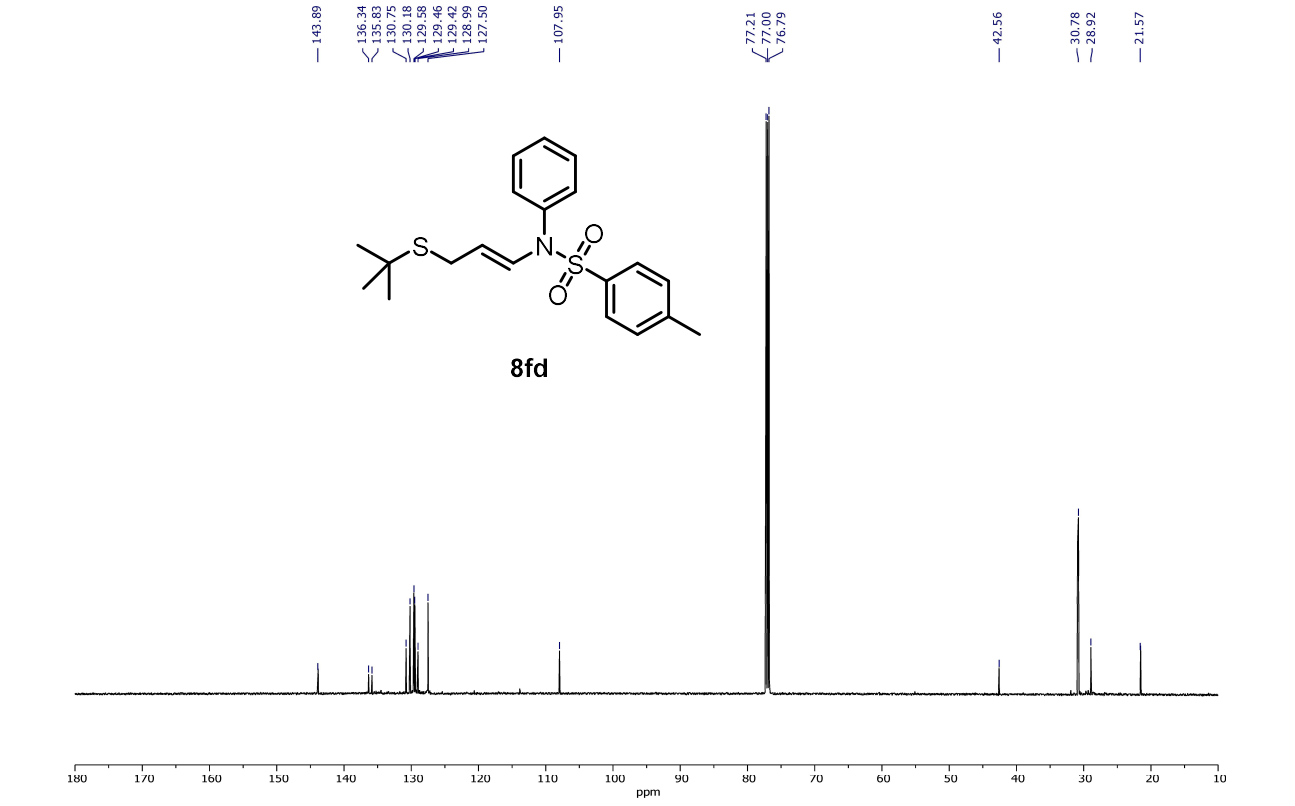
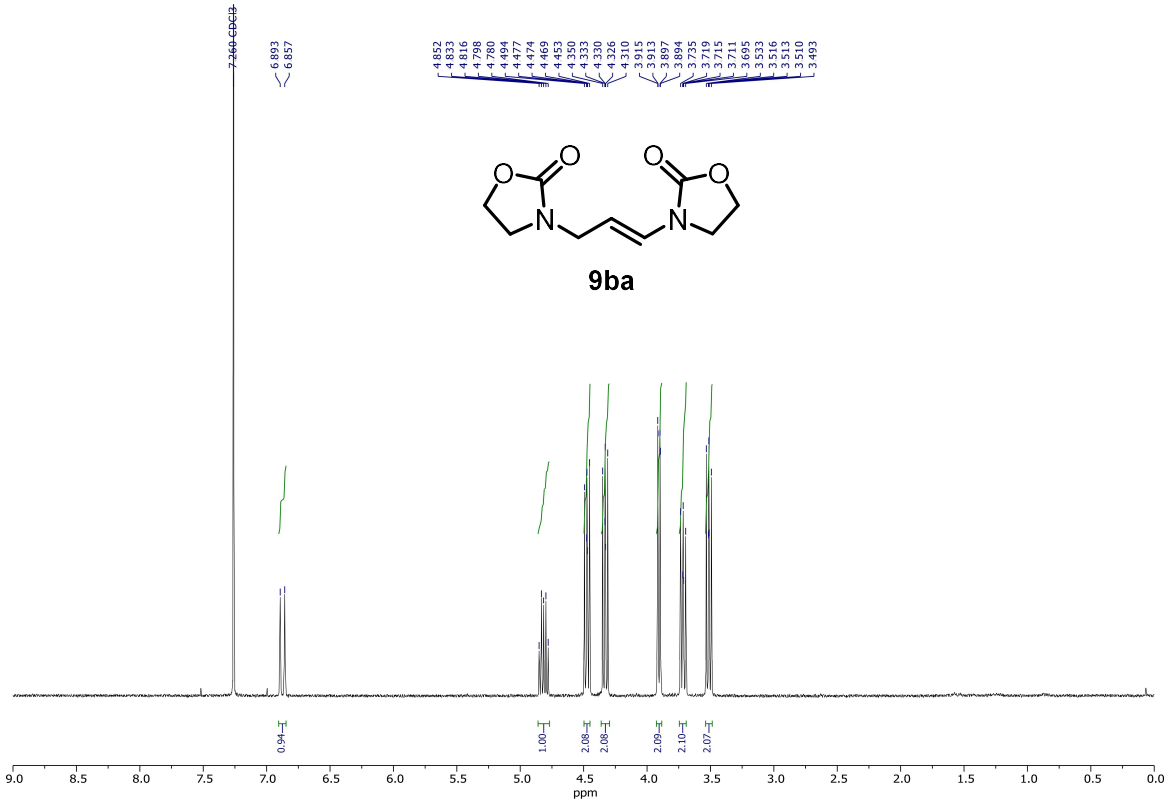
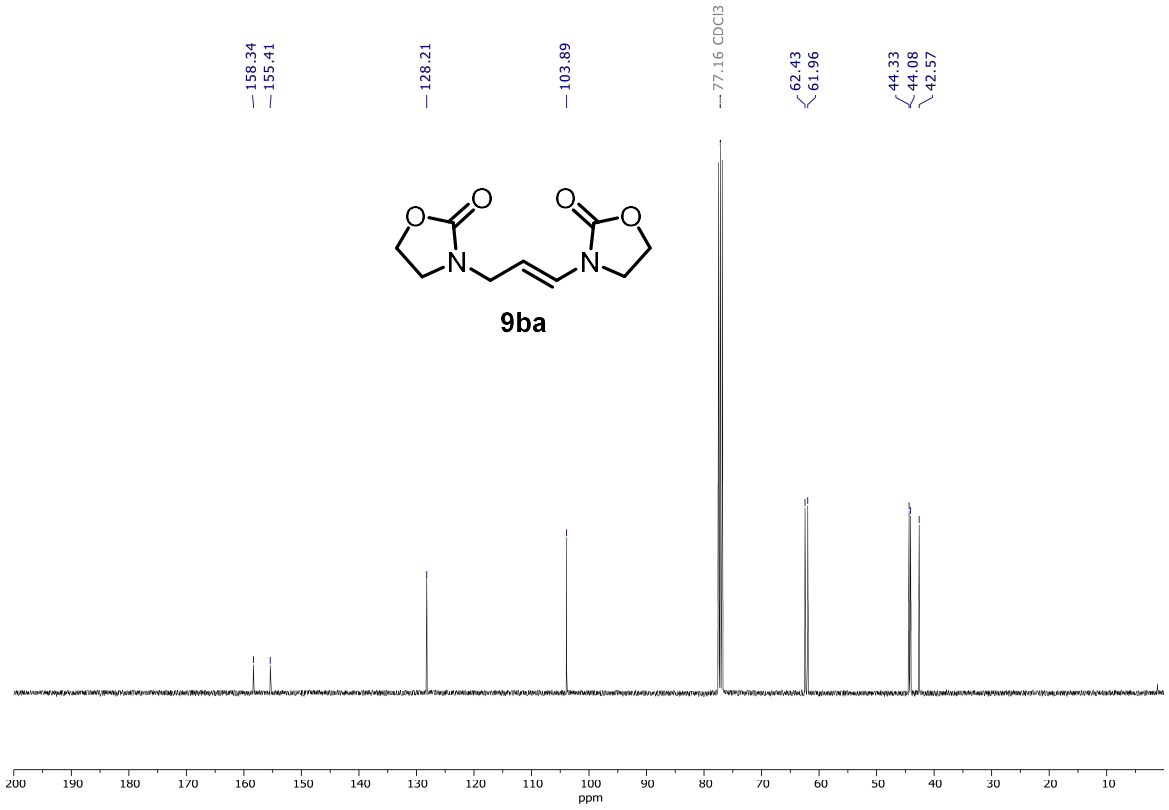


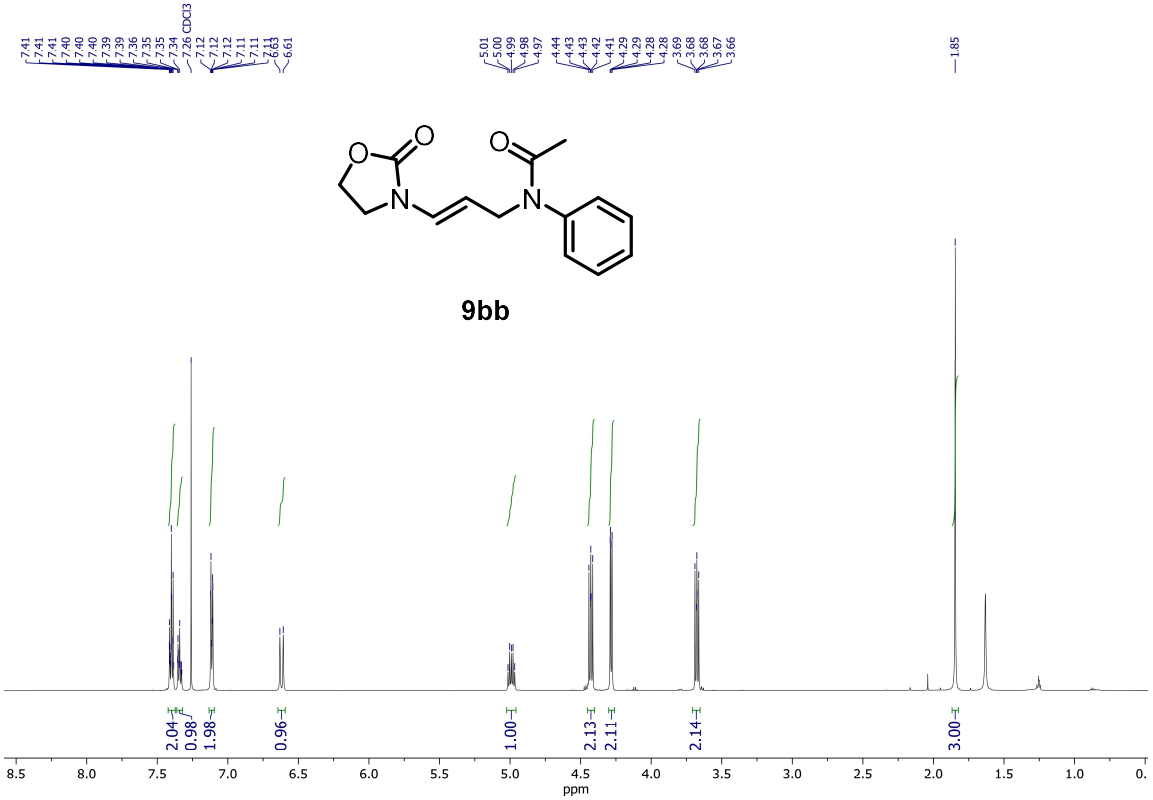
^{1}H NMR (400 MHz, $CDCl_3$)



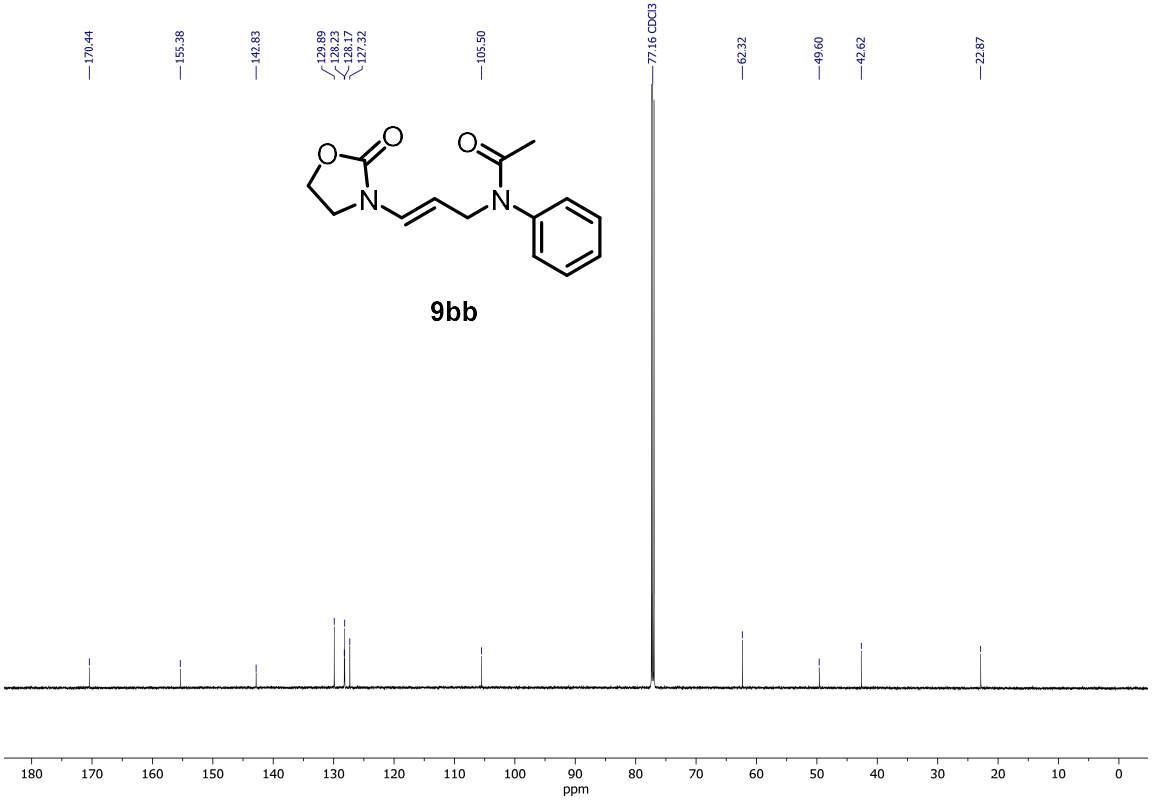
^{13}C NMR (100 MHz, $CDCl_3$)



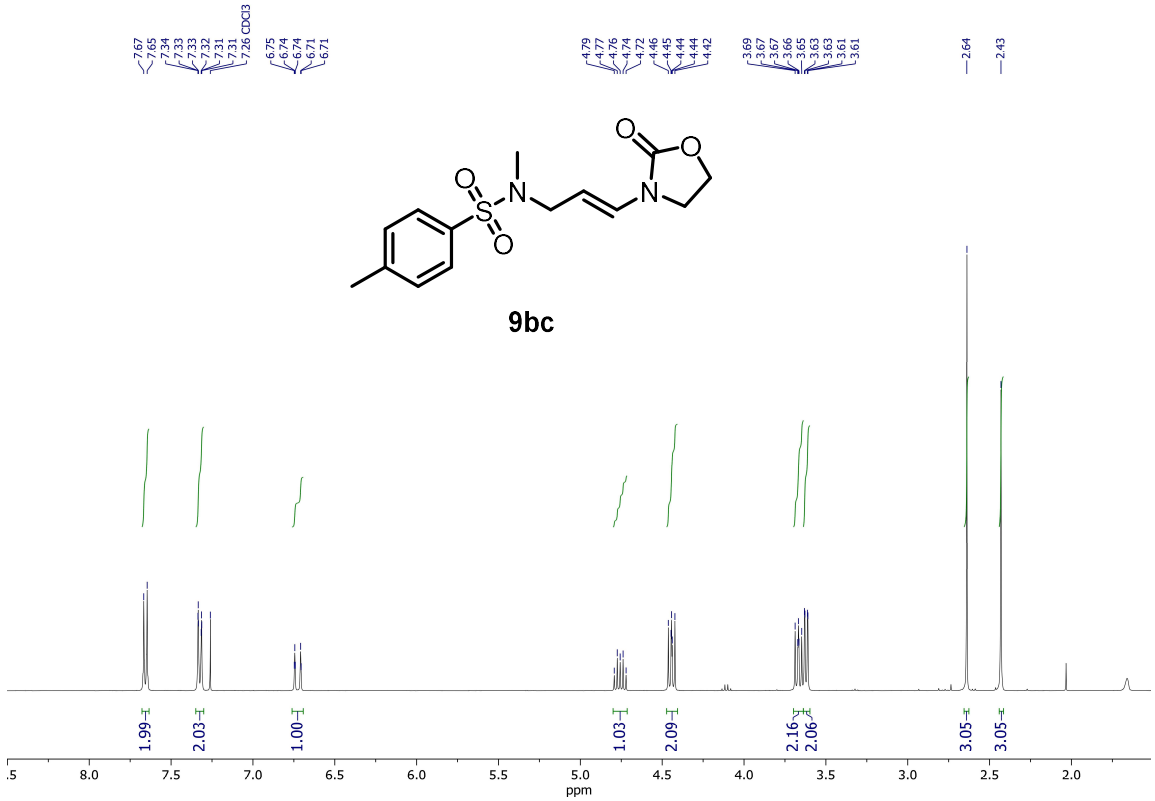
^{1}H NMR (600 MHz, $CDCl_3$)



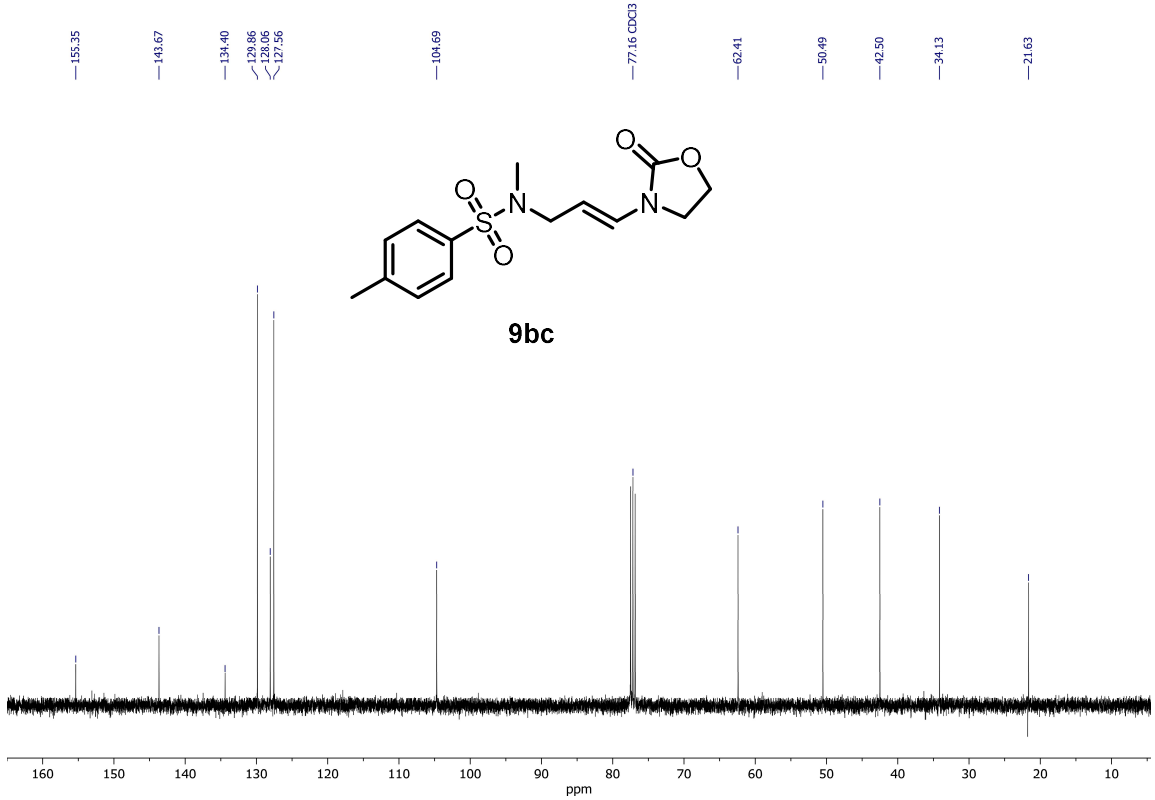
^{13}C NMR (150 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



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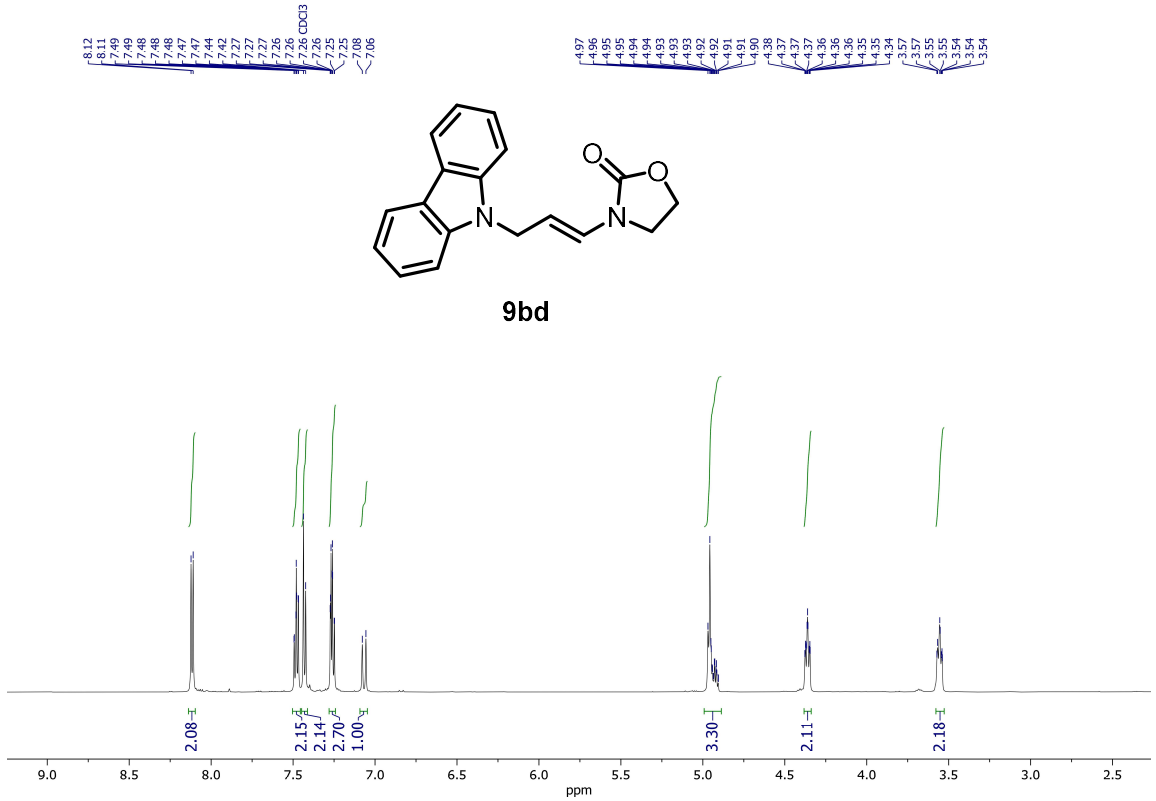
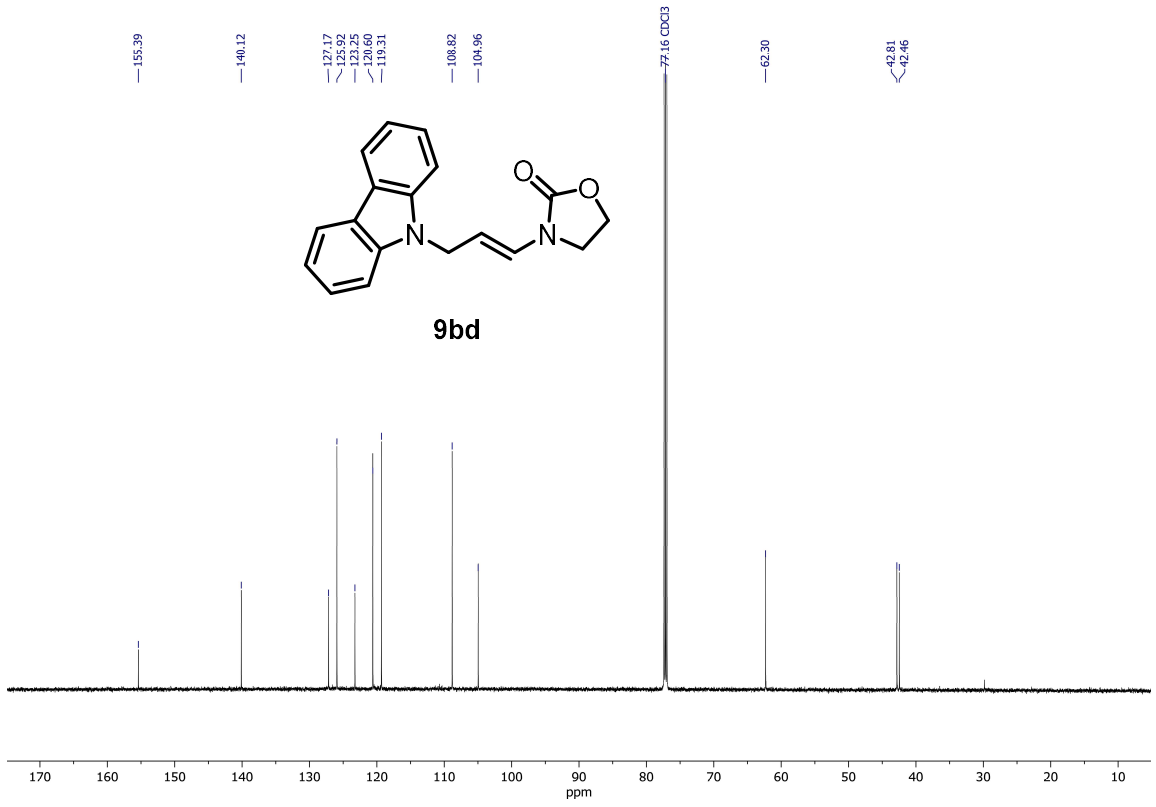


^{13}C NMR (150 MHz, $CDCl_3$)



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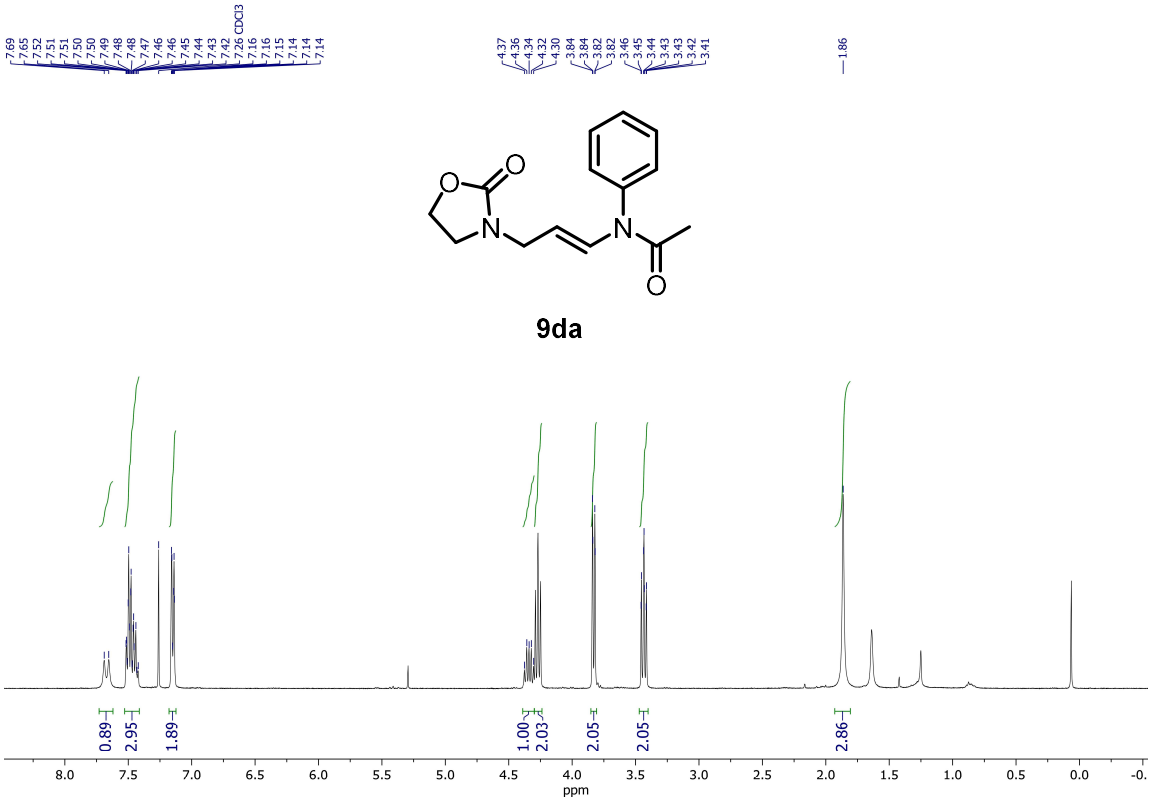
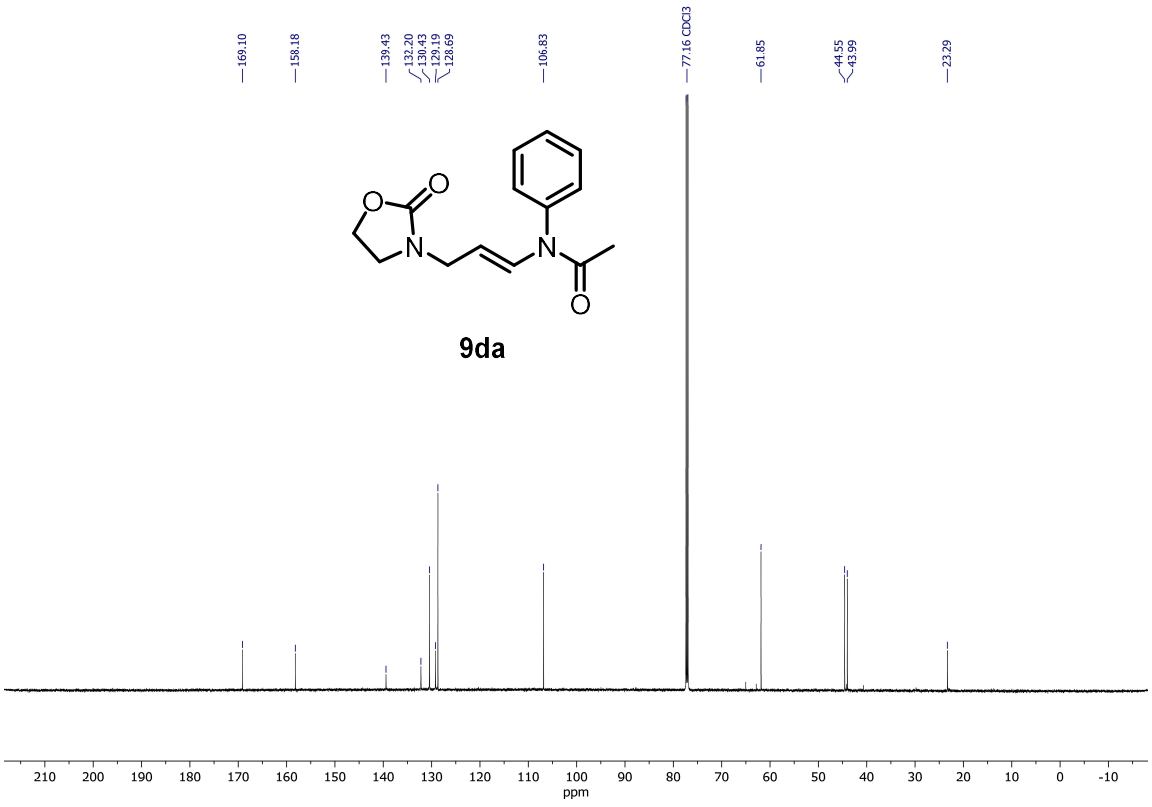
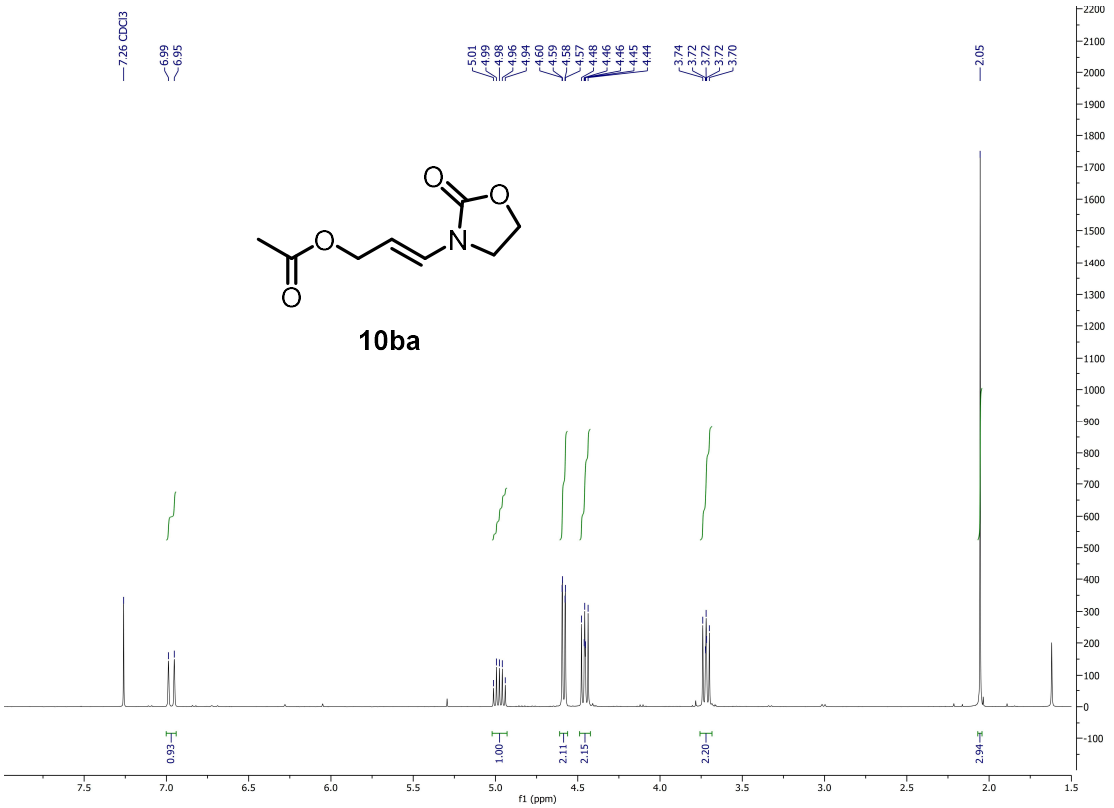


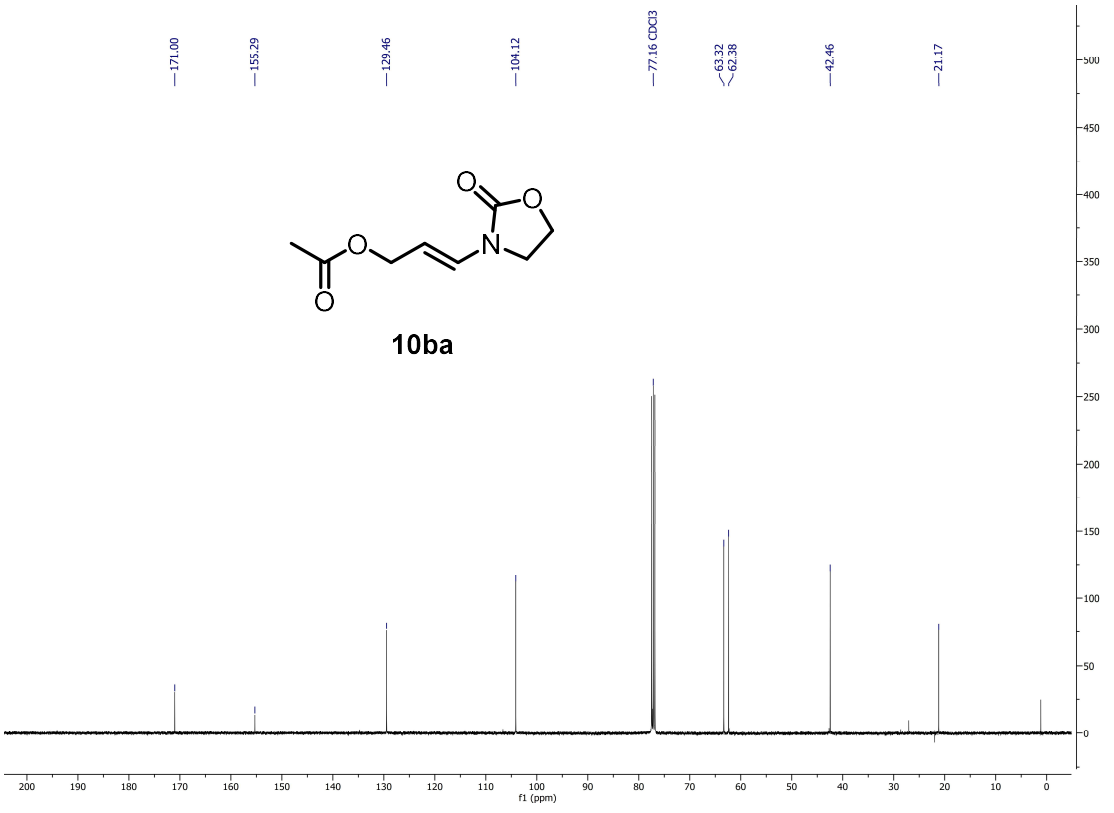
^{13}C NMR (150 MHz, $CDCl_3$)



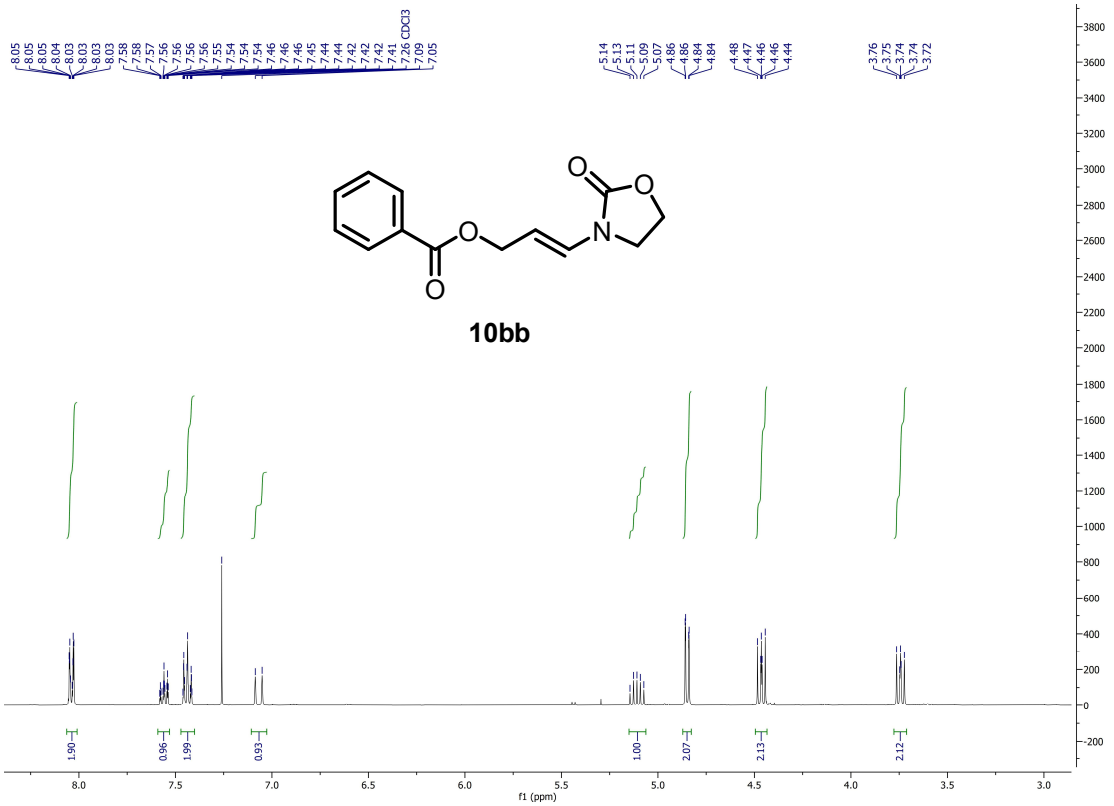
^{1}H NMR (400 MHz, $CDCl_3$)



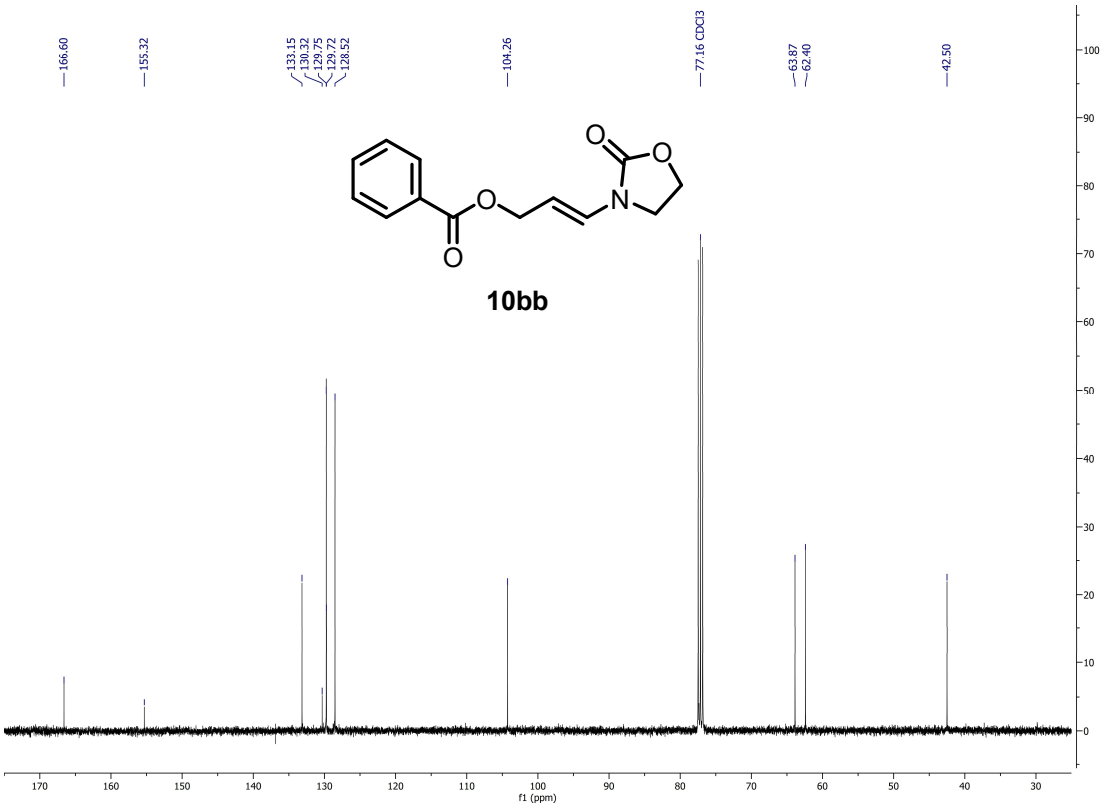
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



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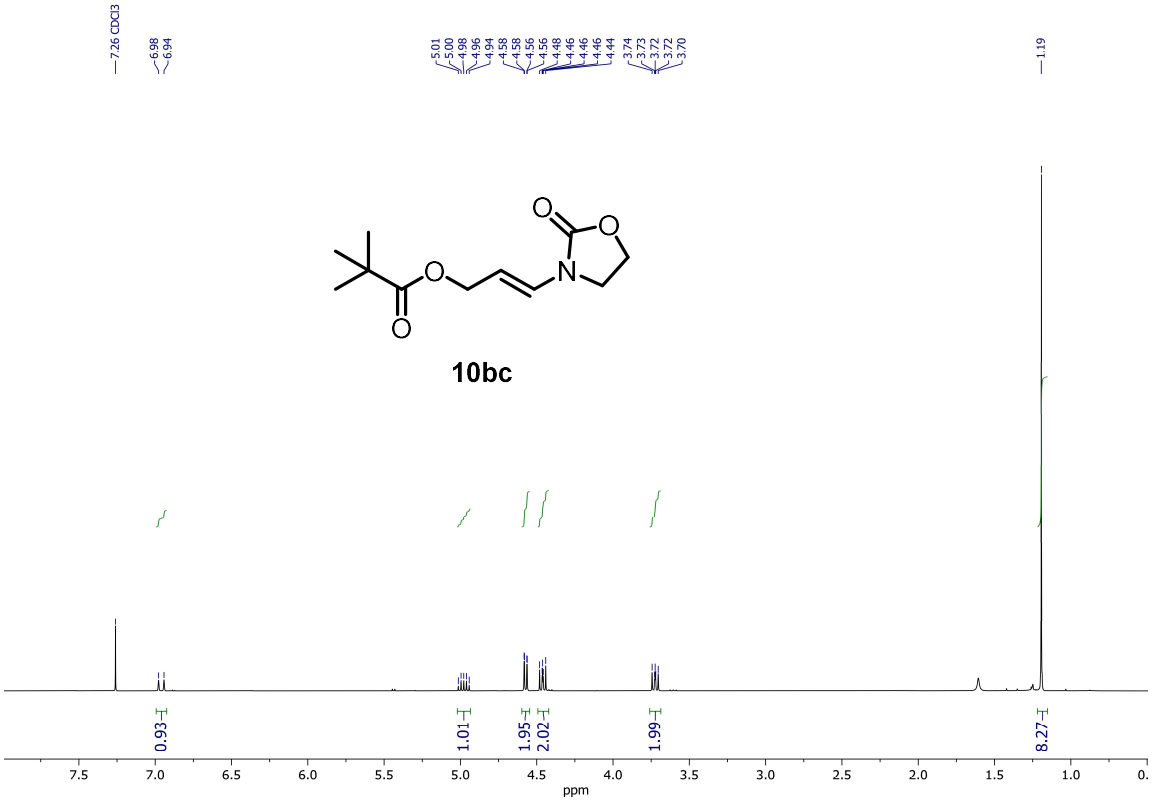

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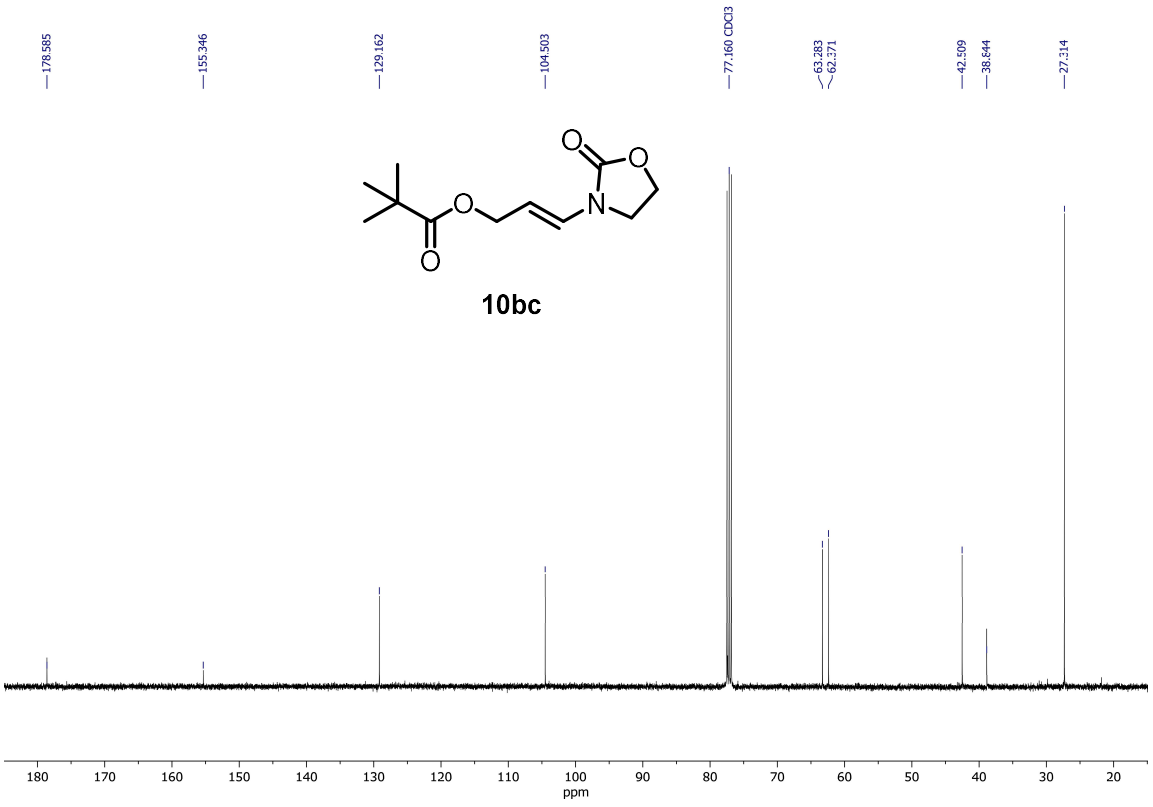

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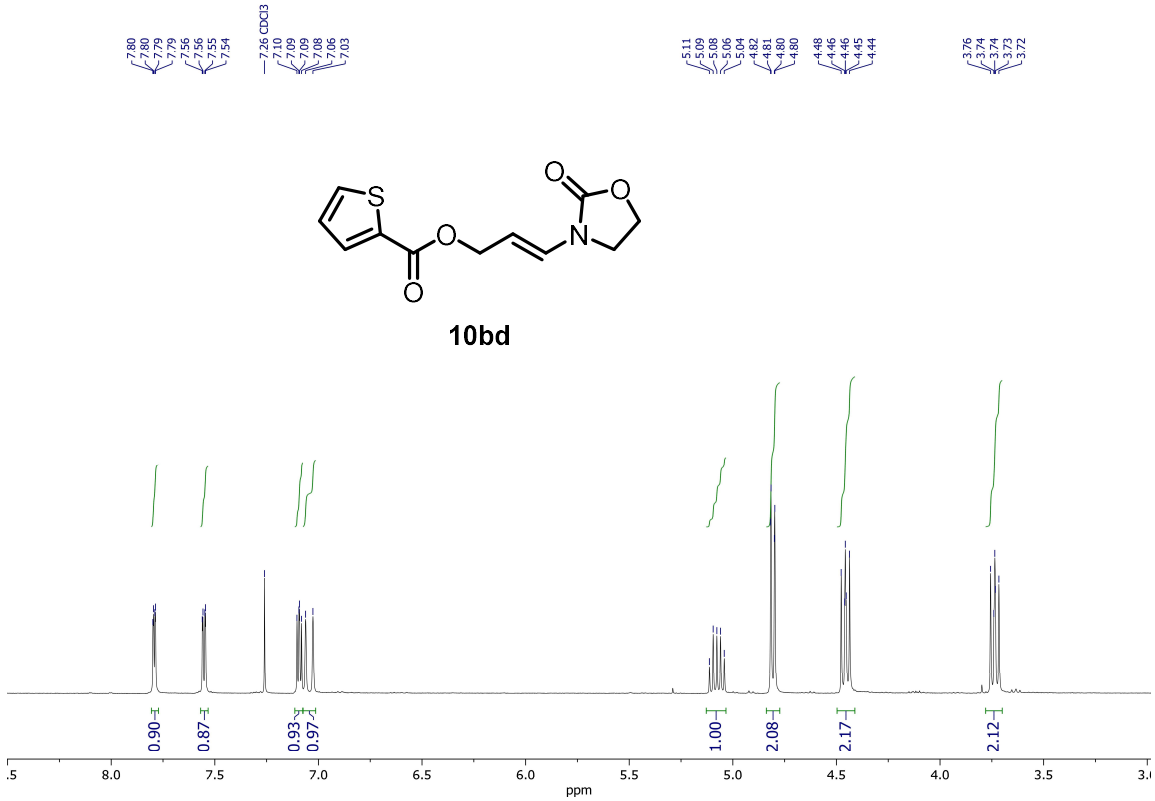
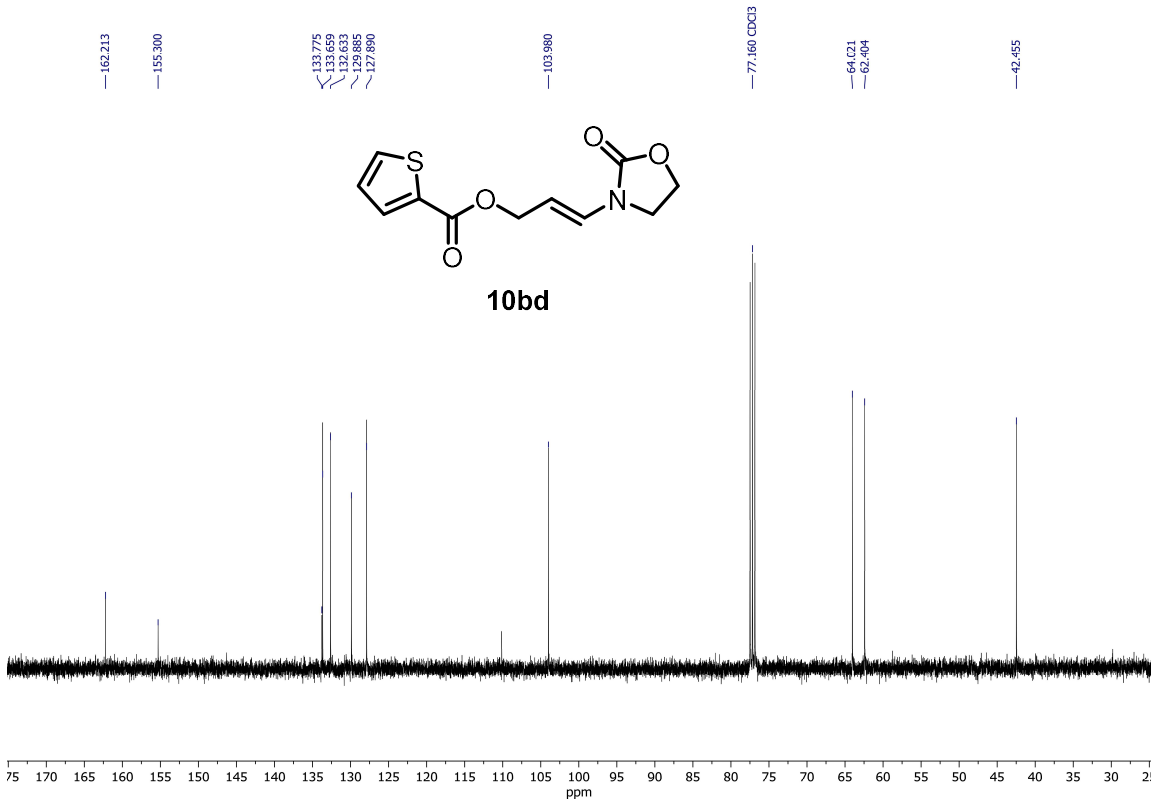


^{13}C NMR (100 MHz, $CDCl_3$)



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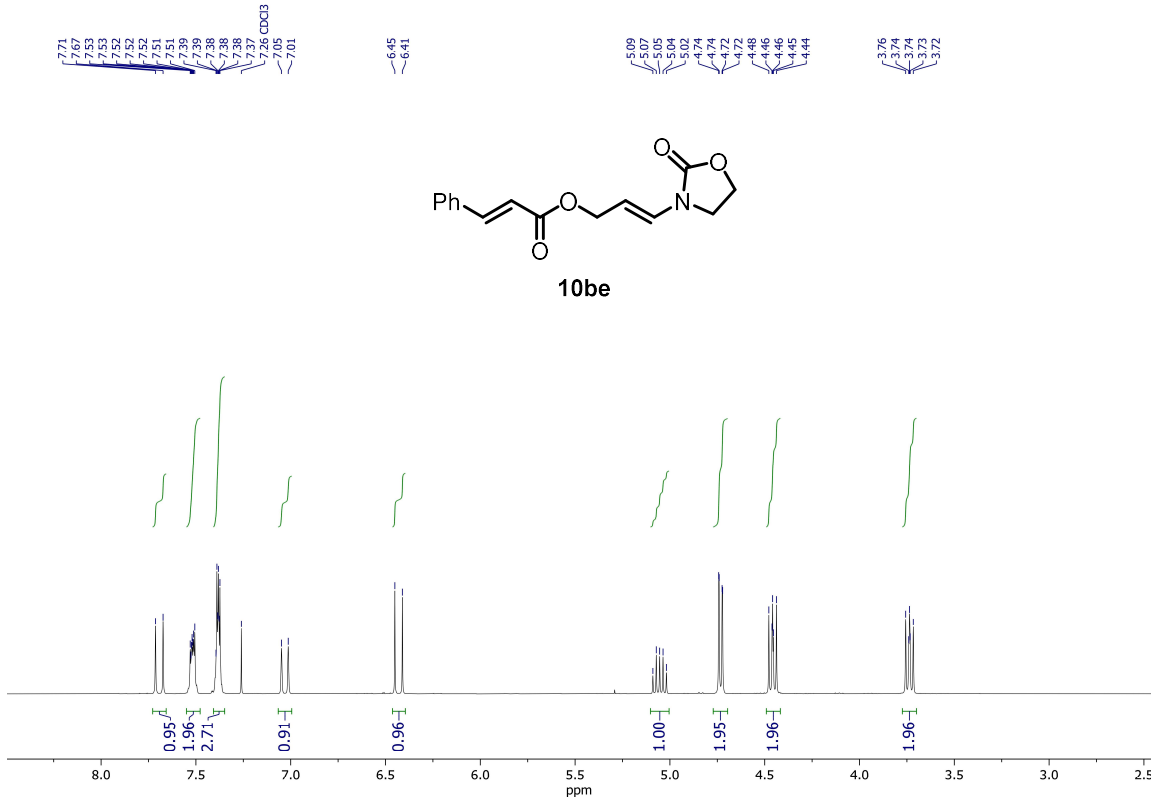

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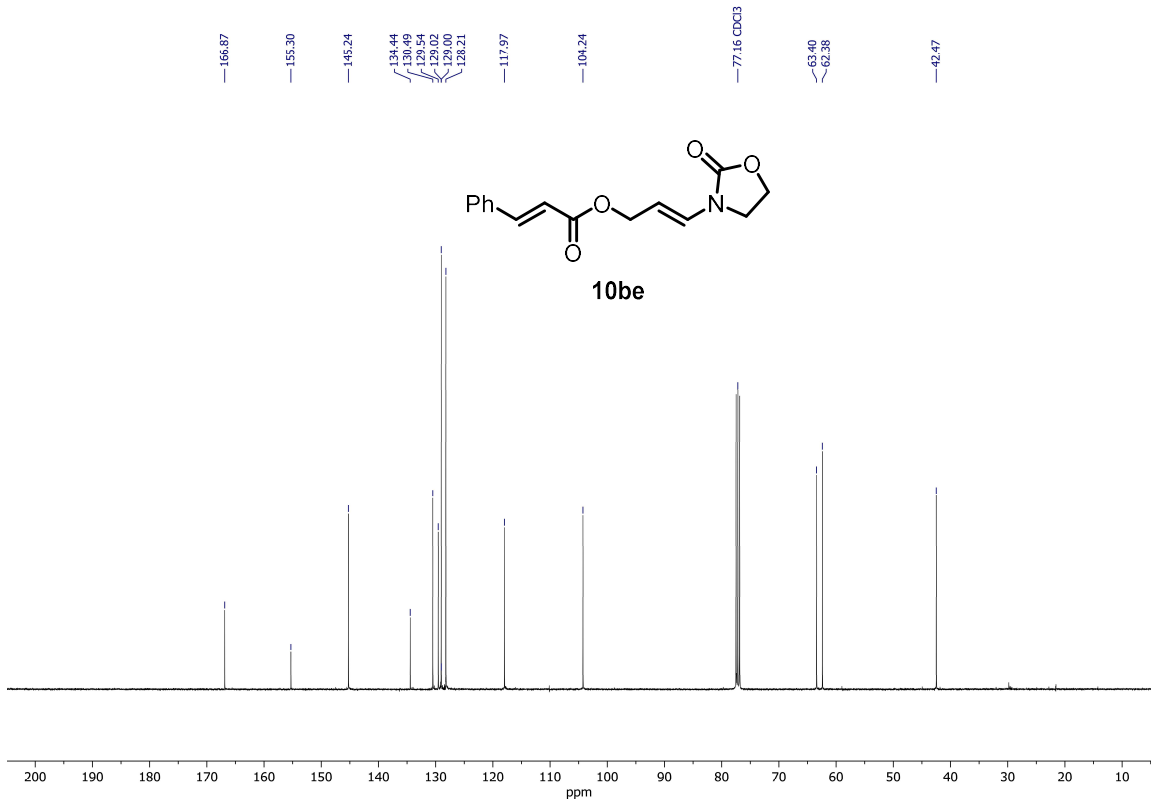

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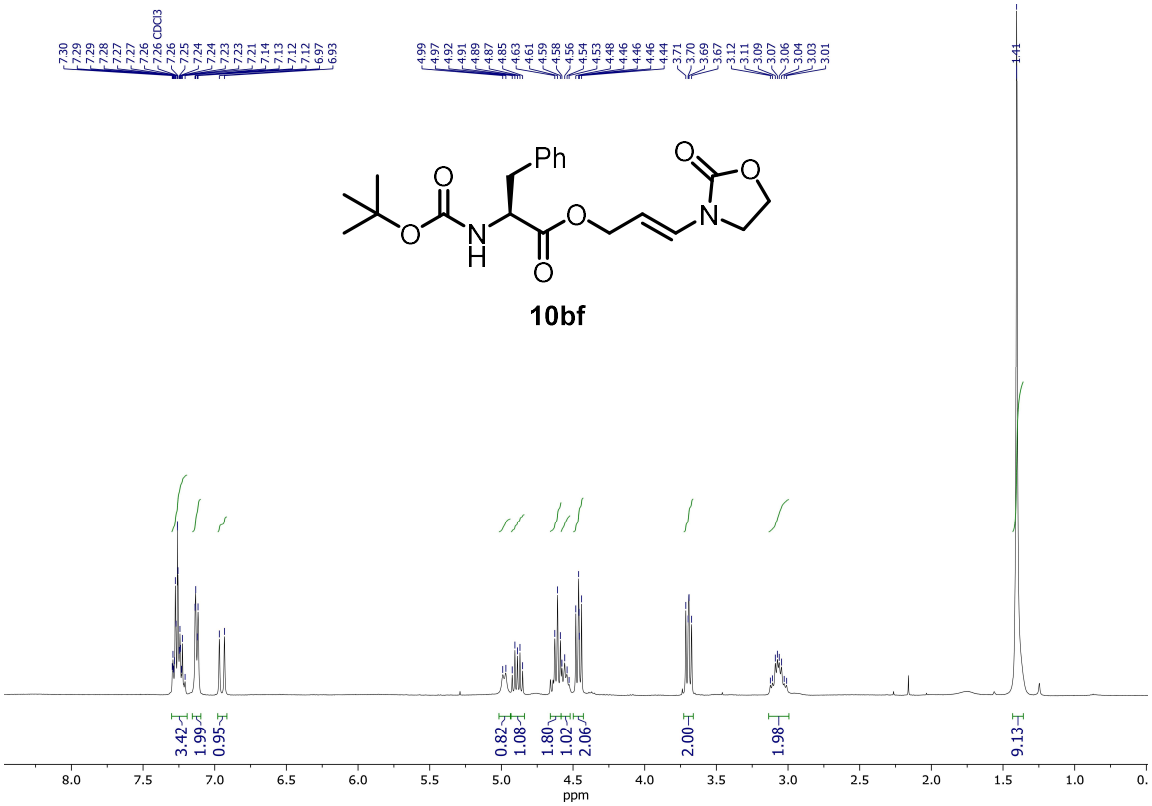

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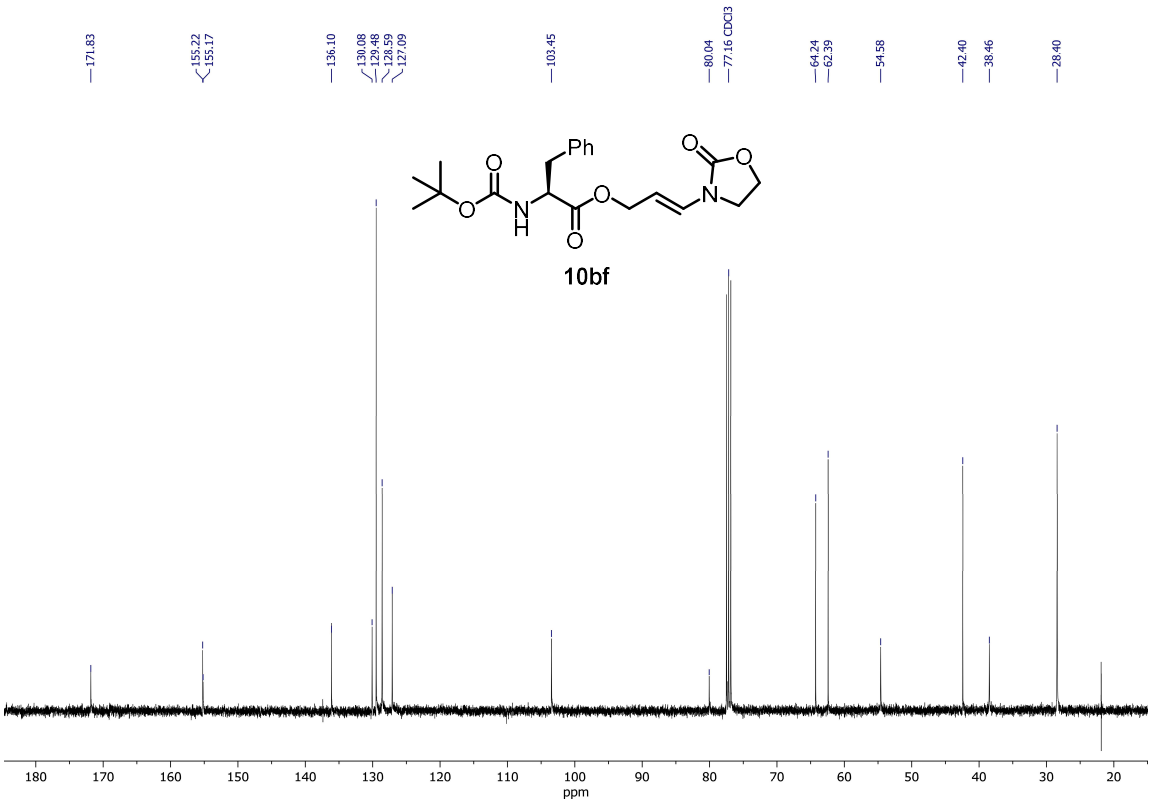

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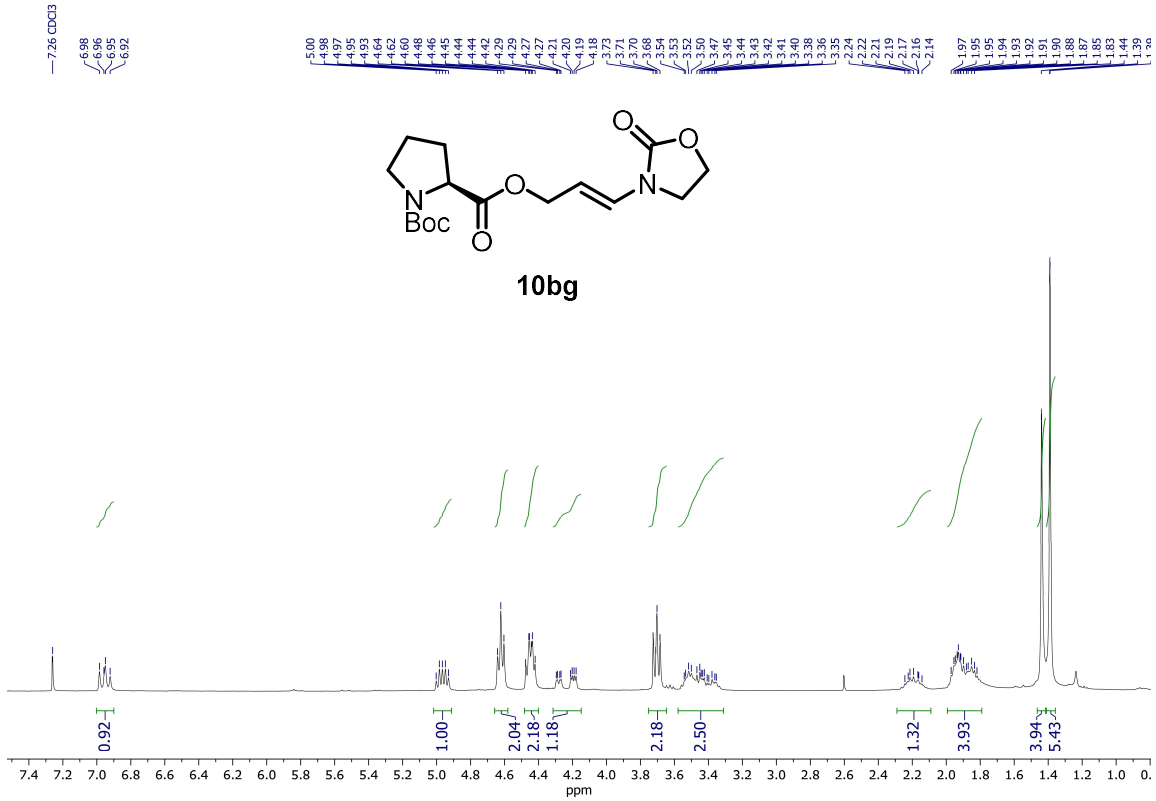

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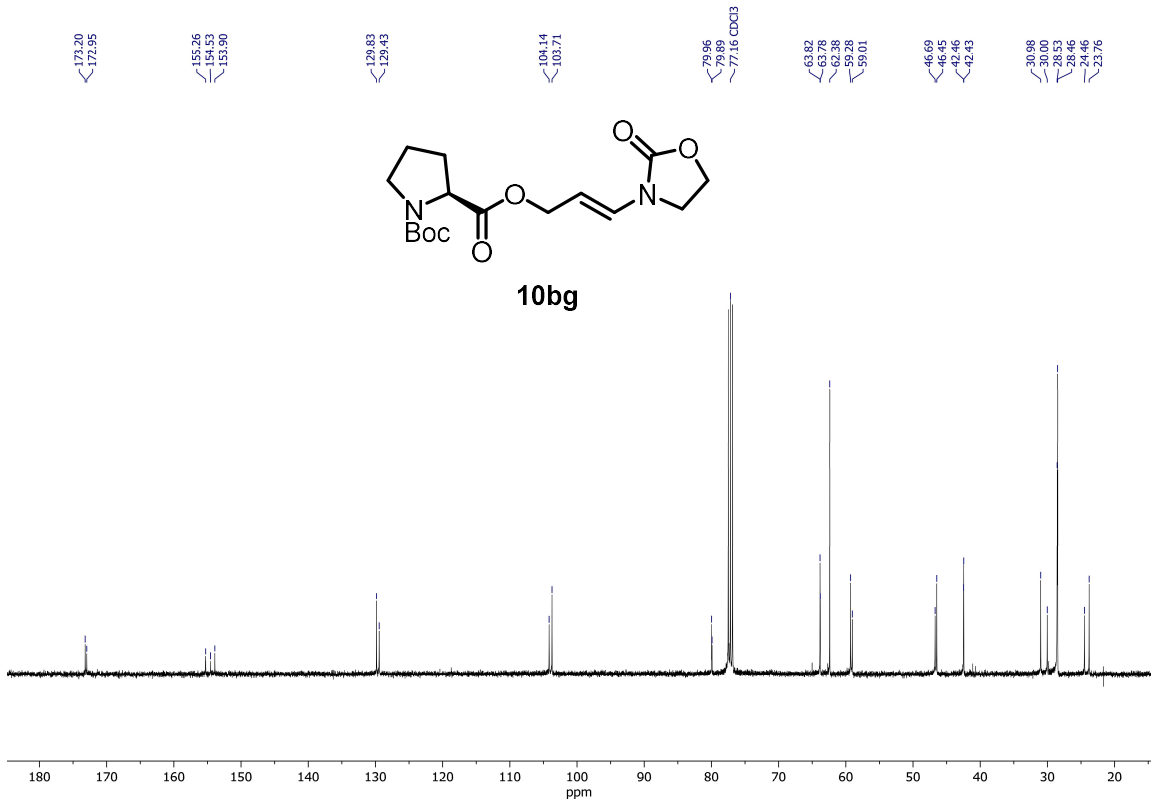

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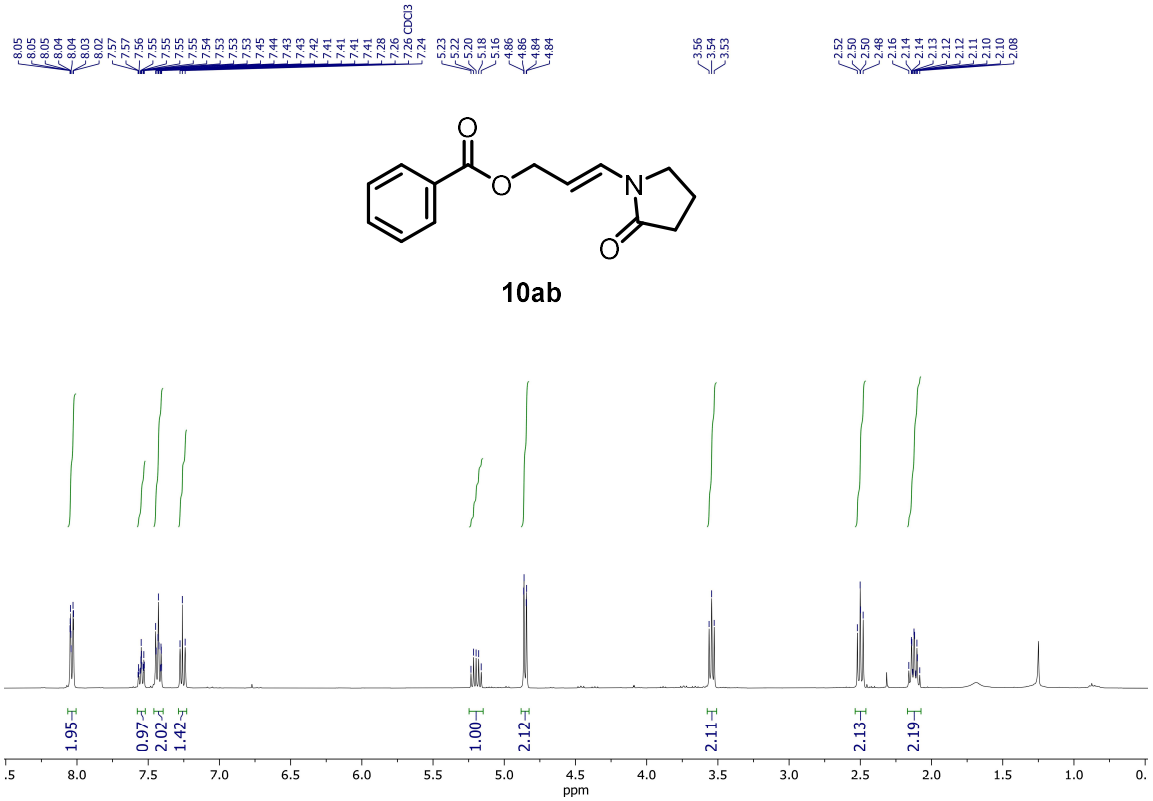

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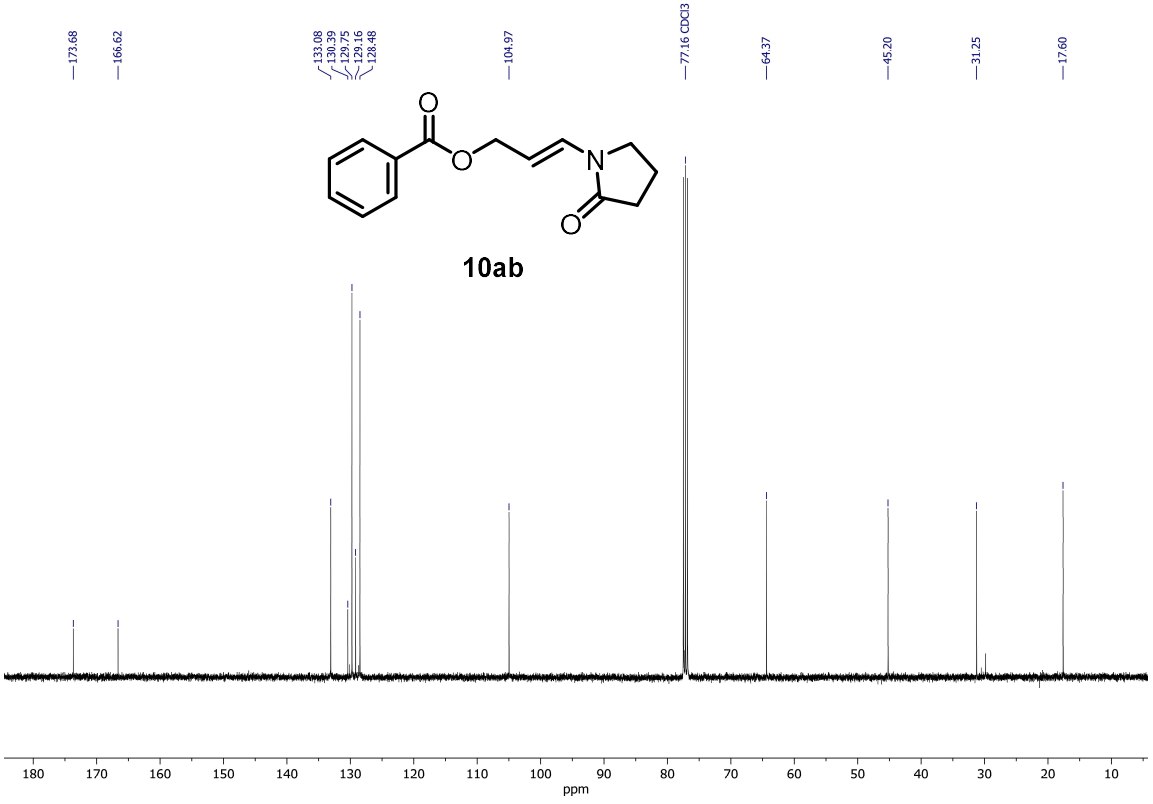

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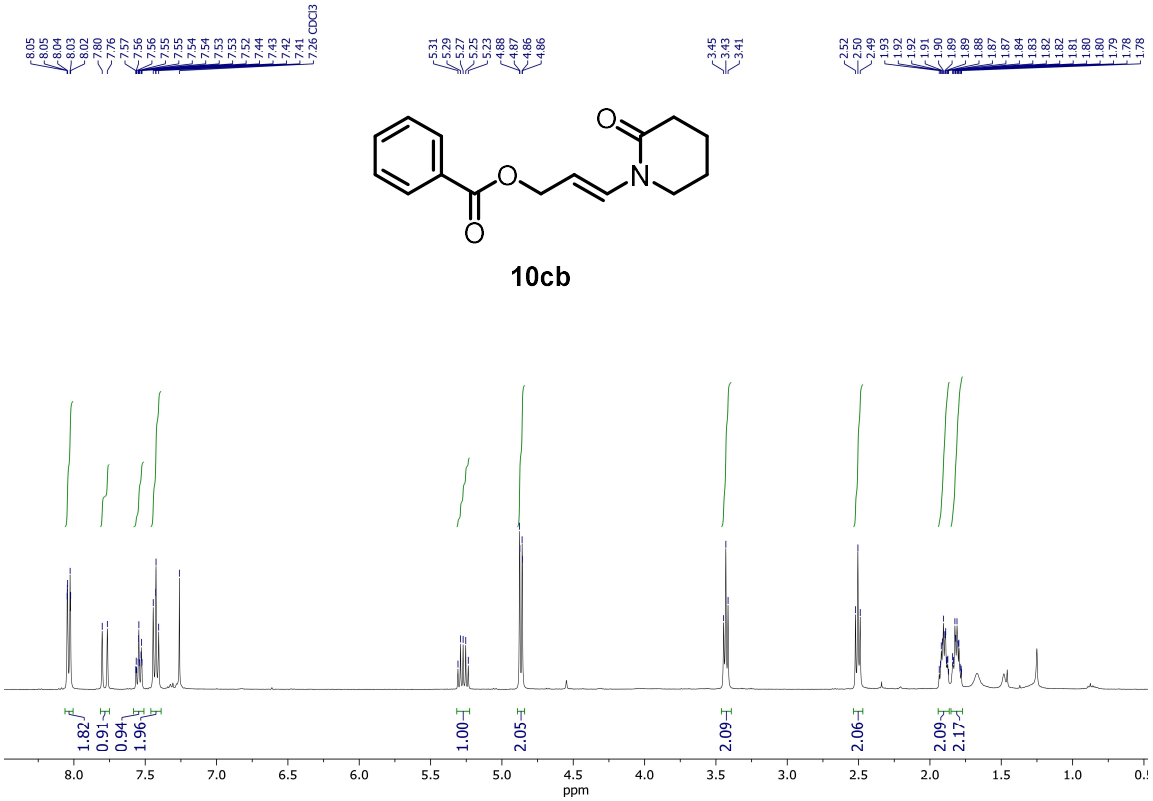
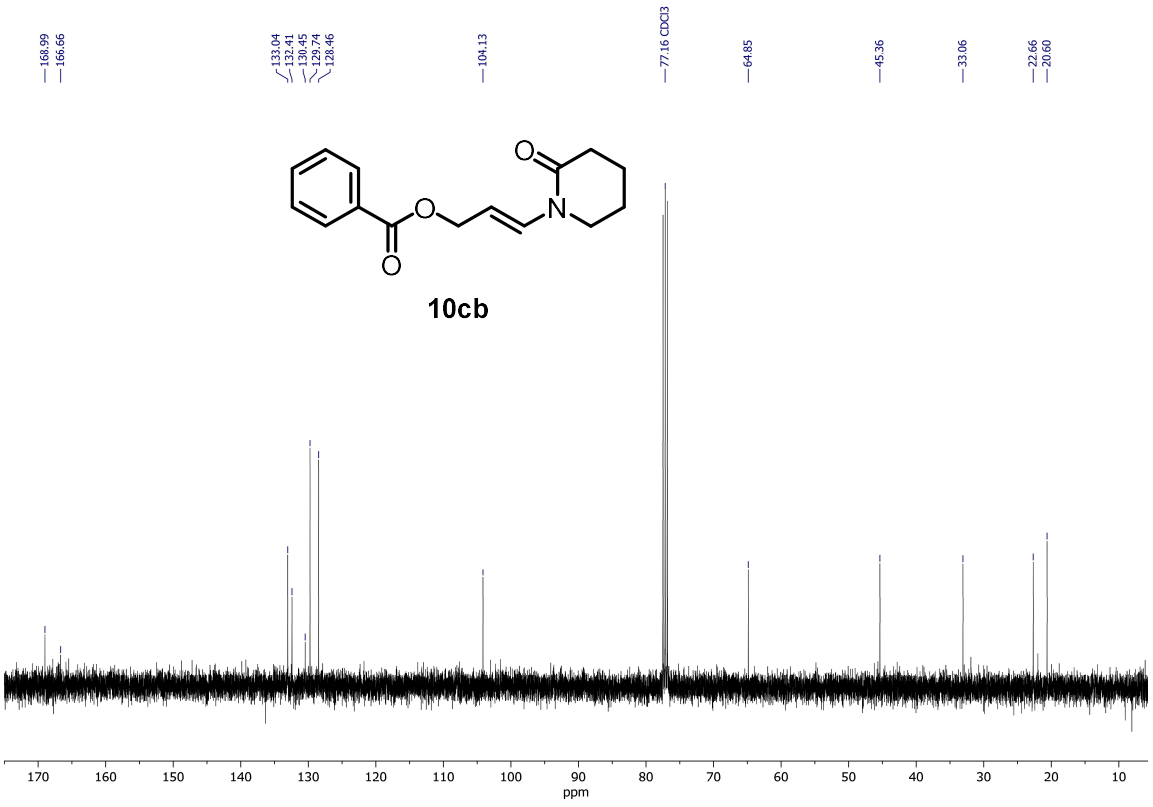


^{13}C NMR (100 MHz, $CDCl_3$)



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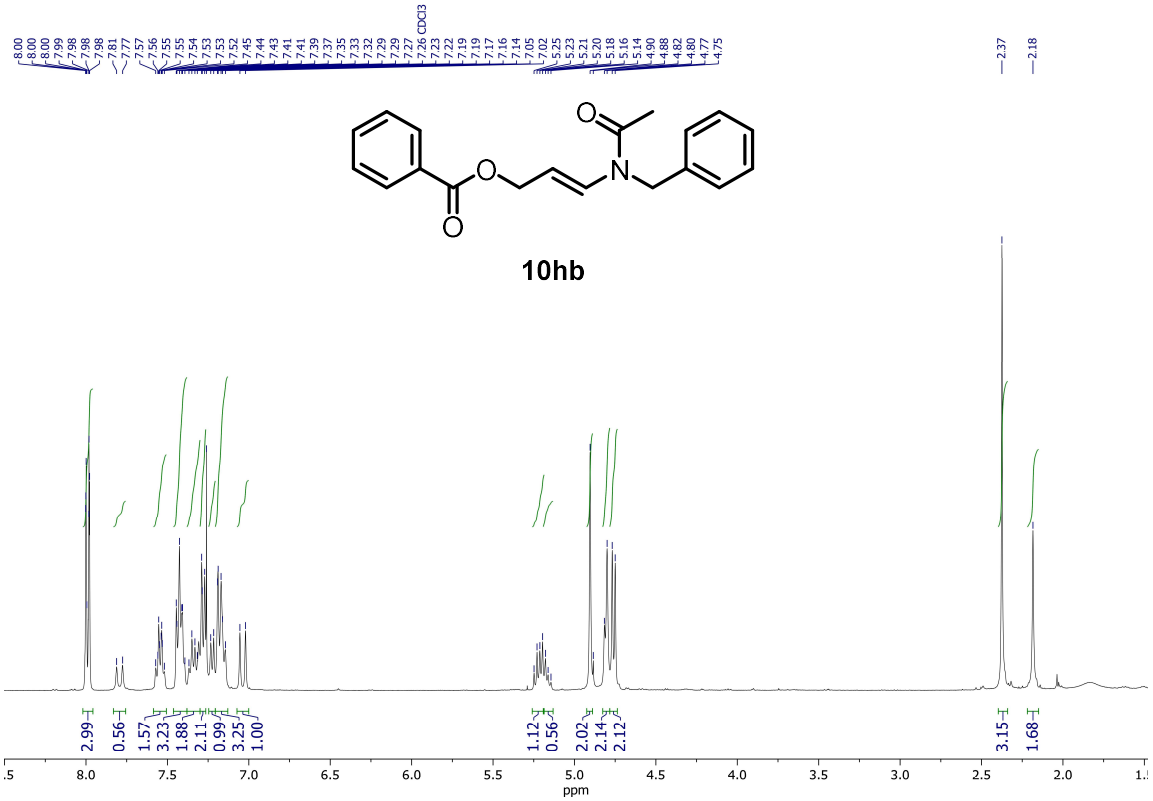
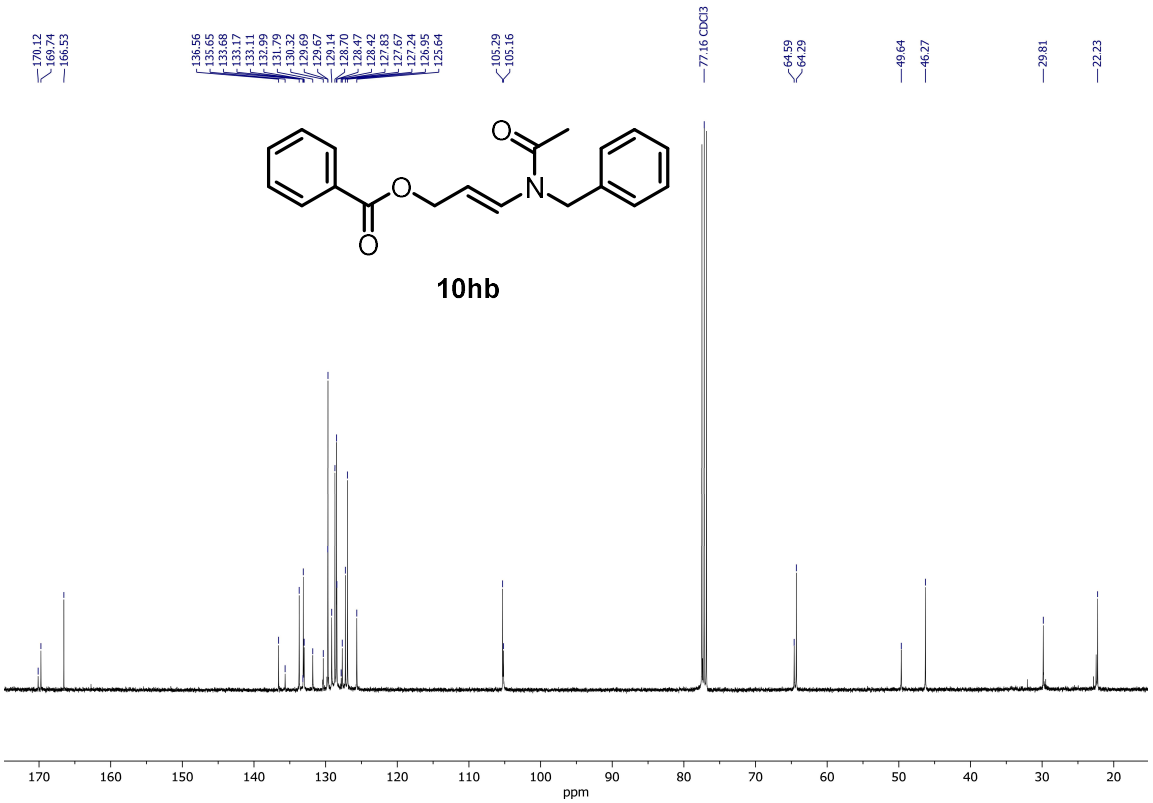


^{13}C NMR (100 MHz, $CDCl_3$)



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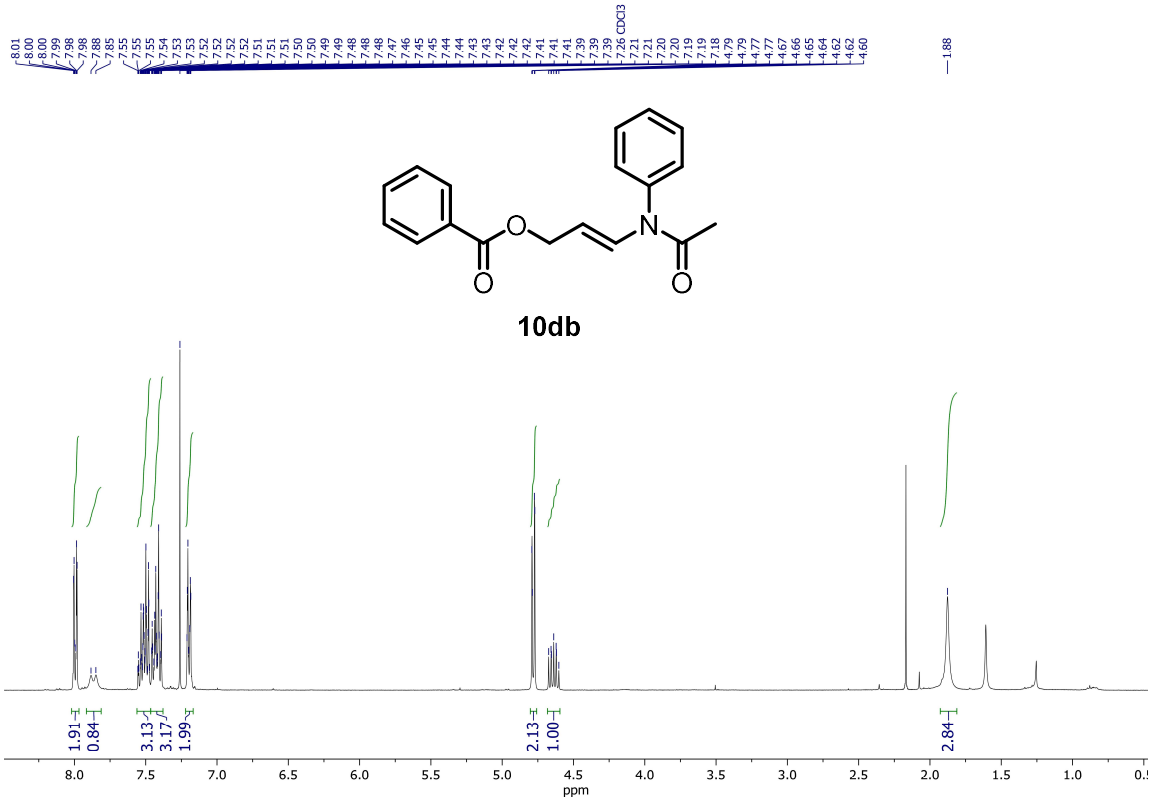
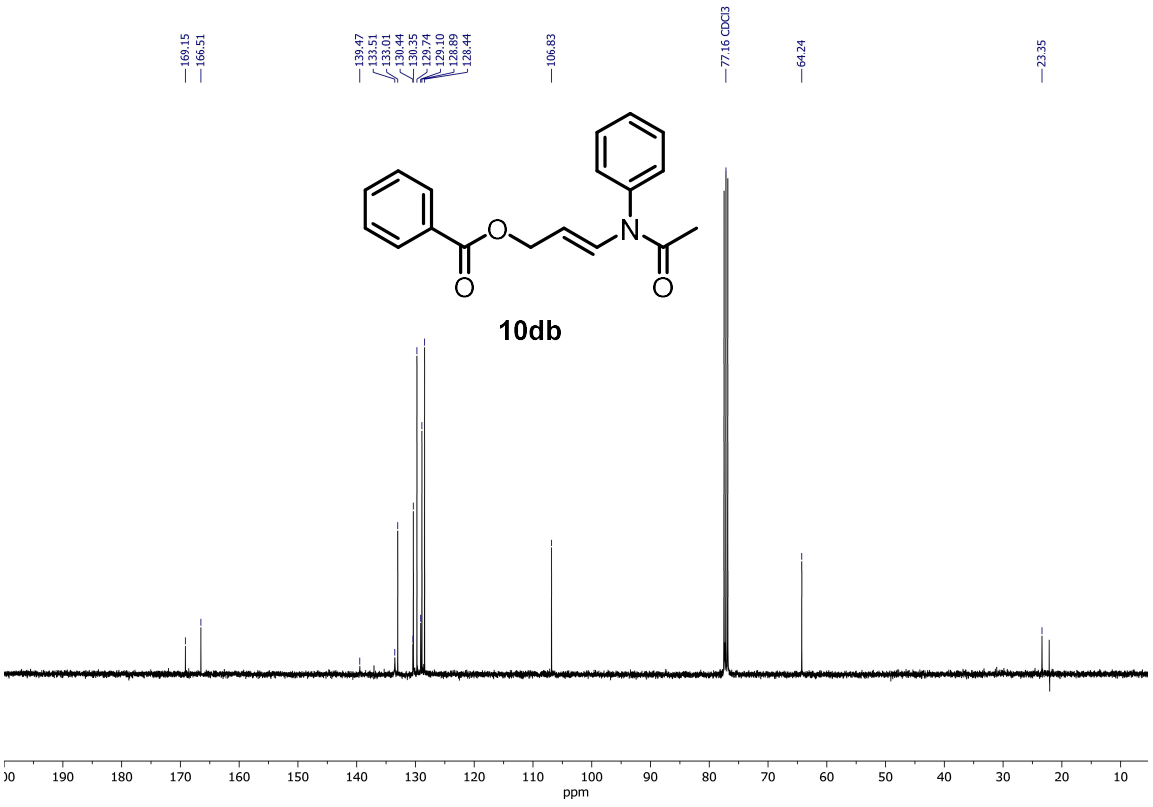
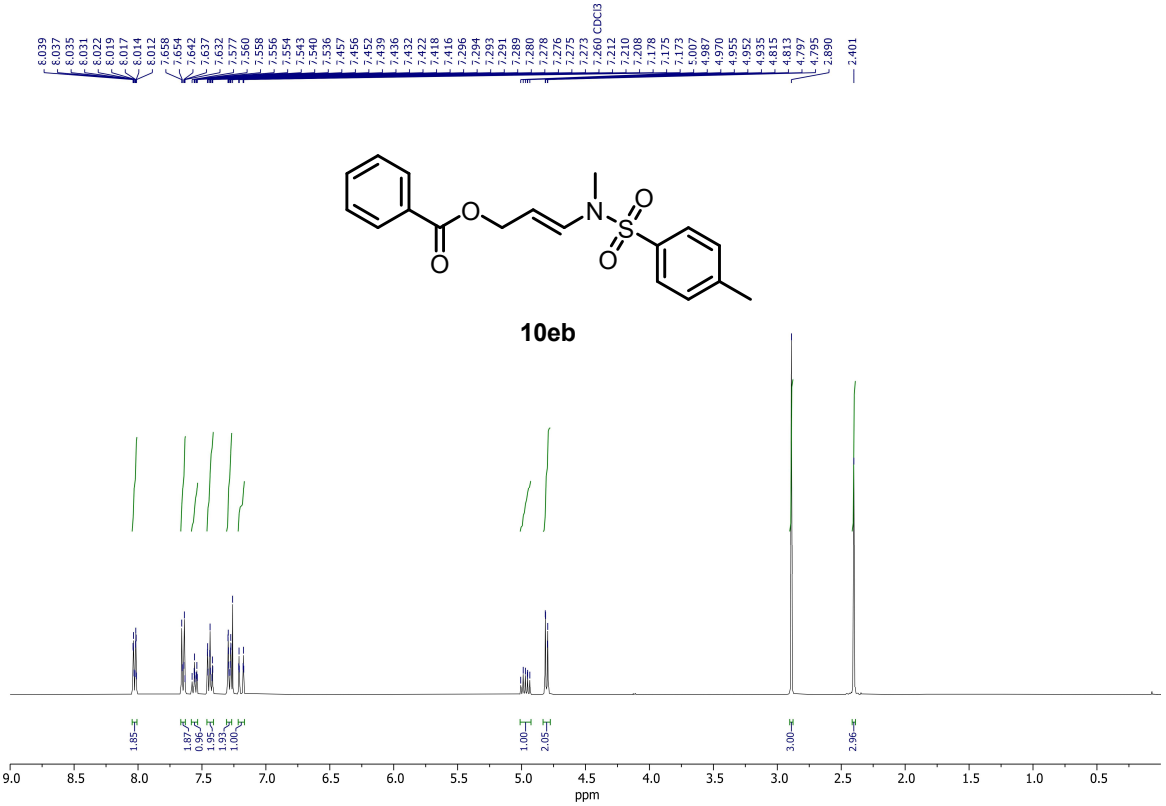


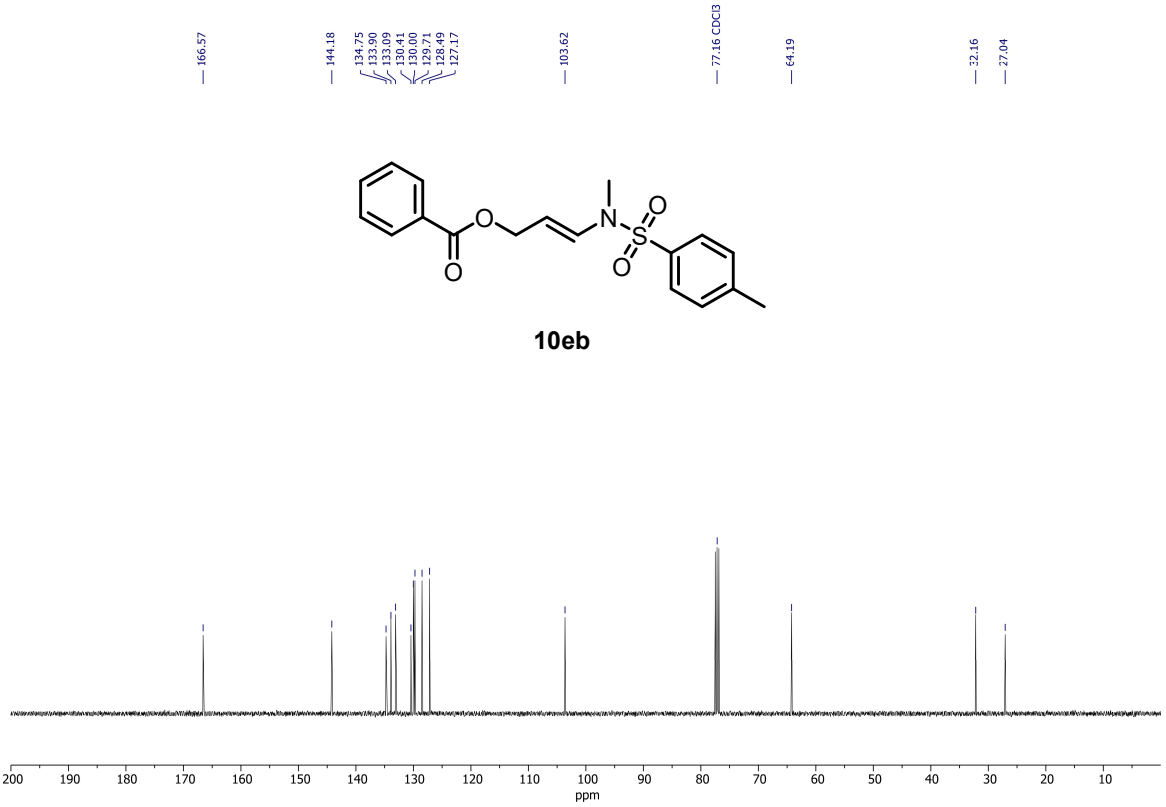
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



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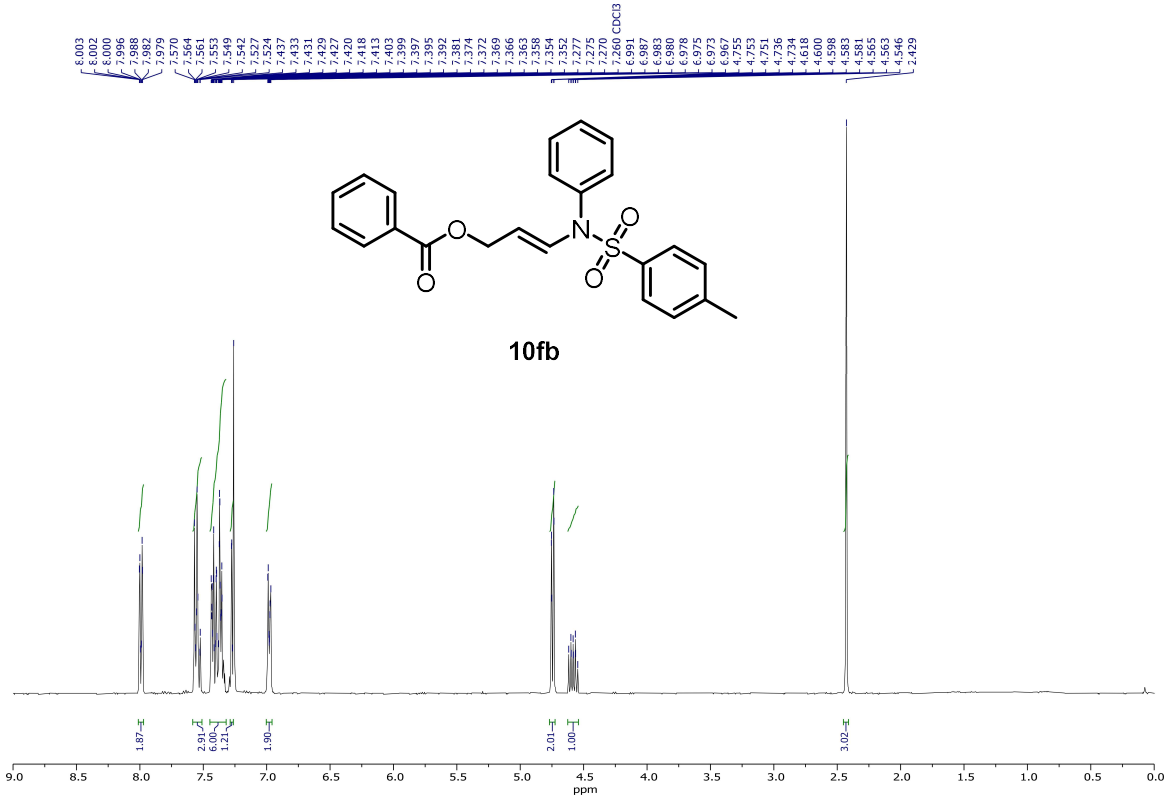

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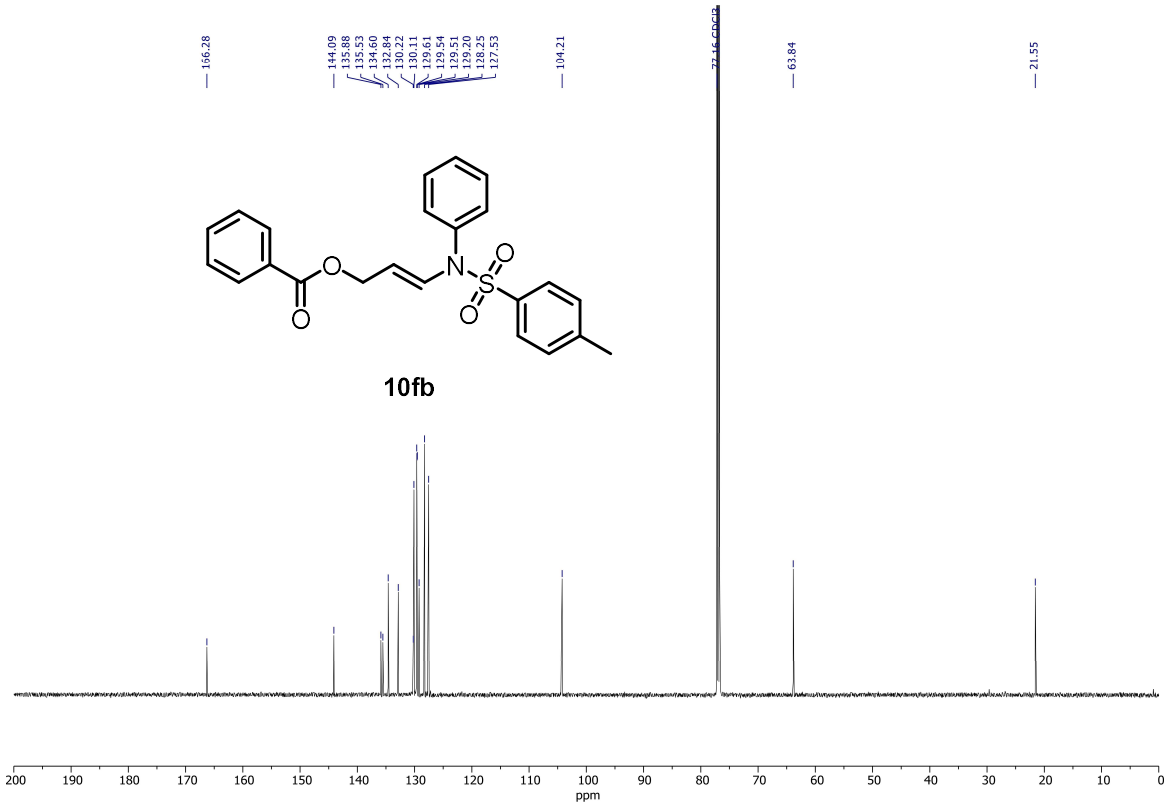

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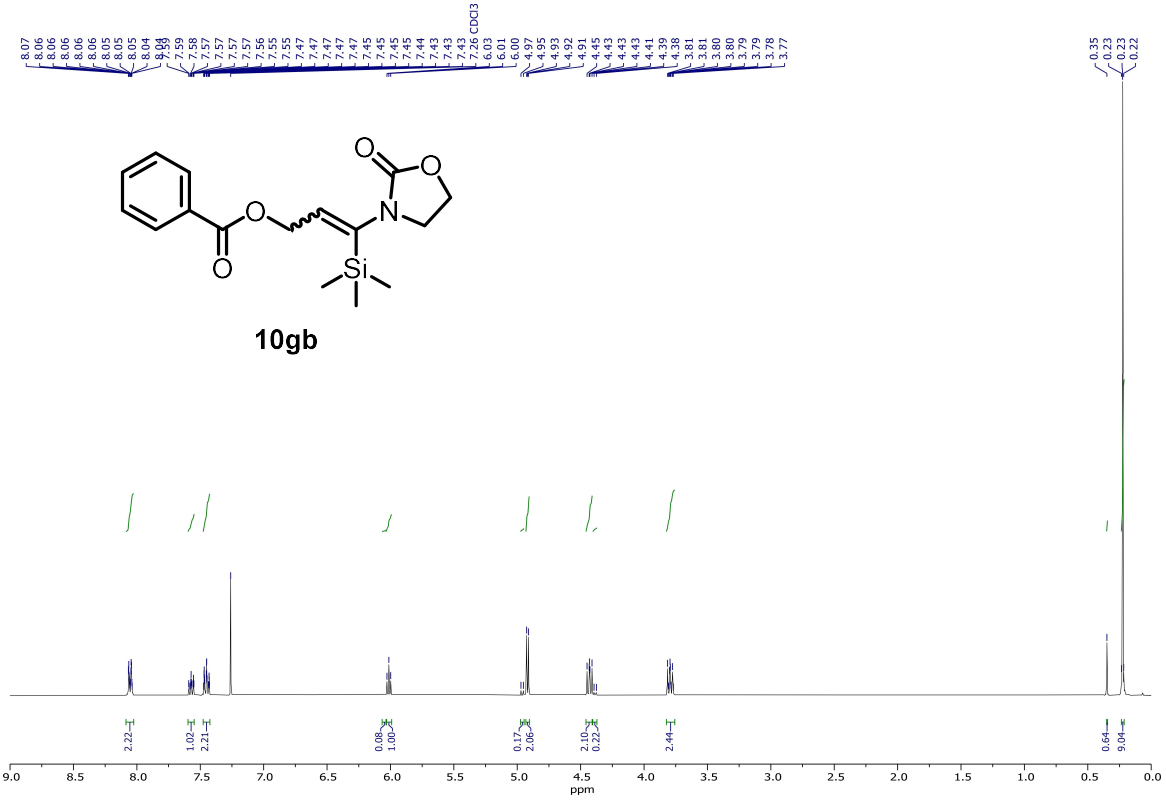

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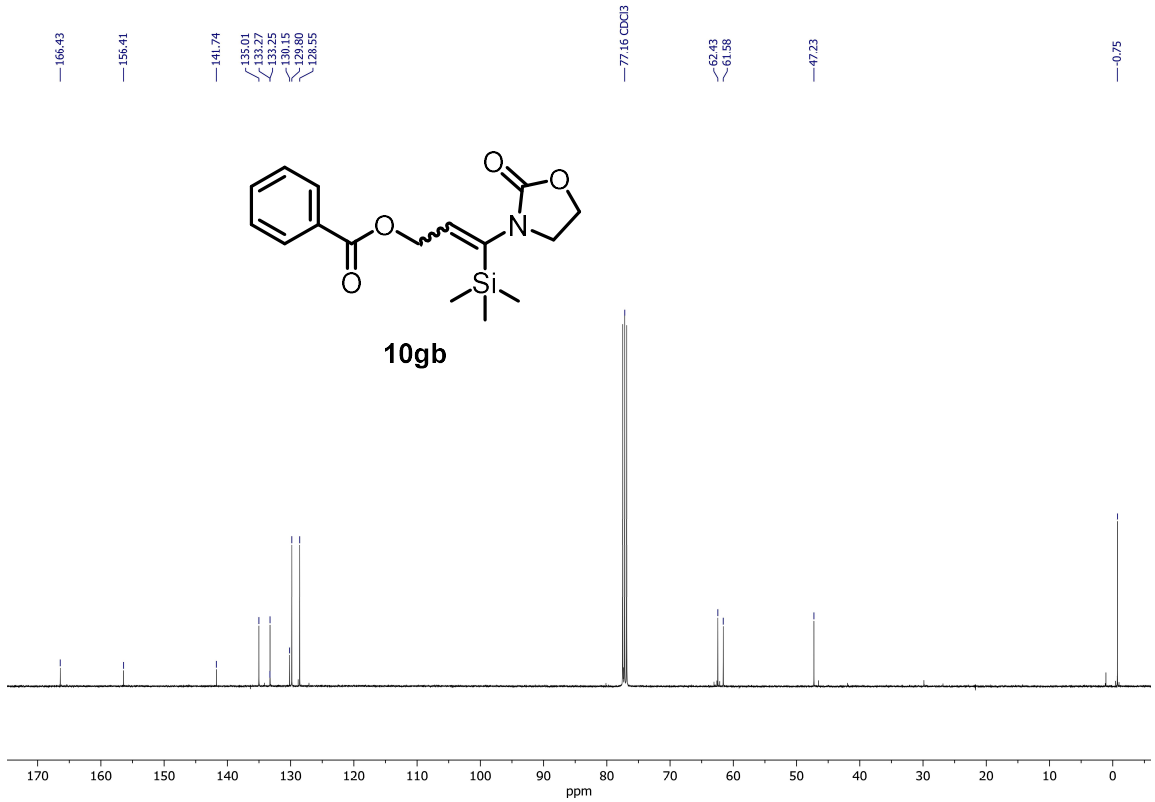
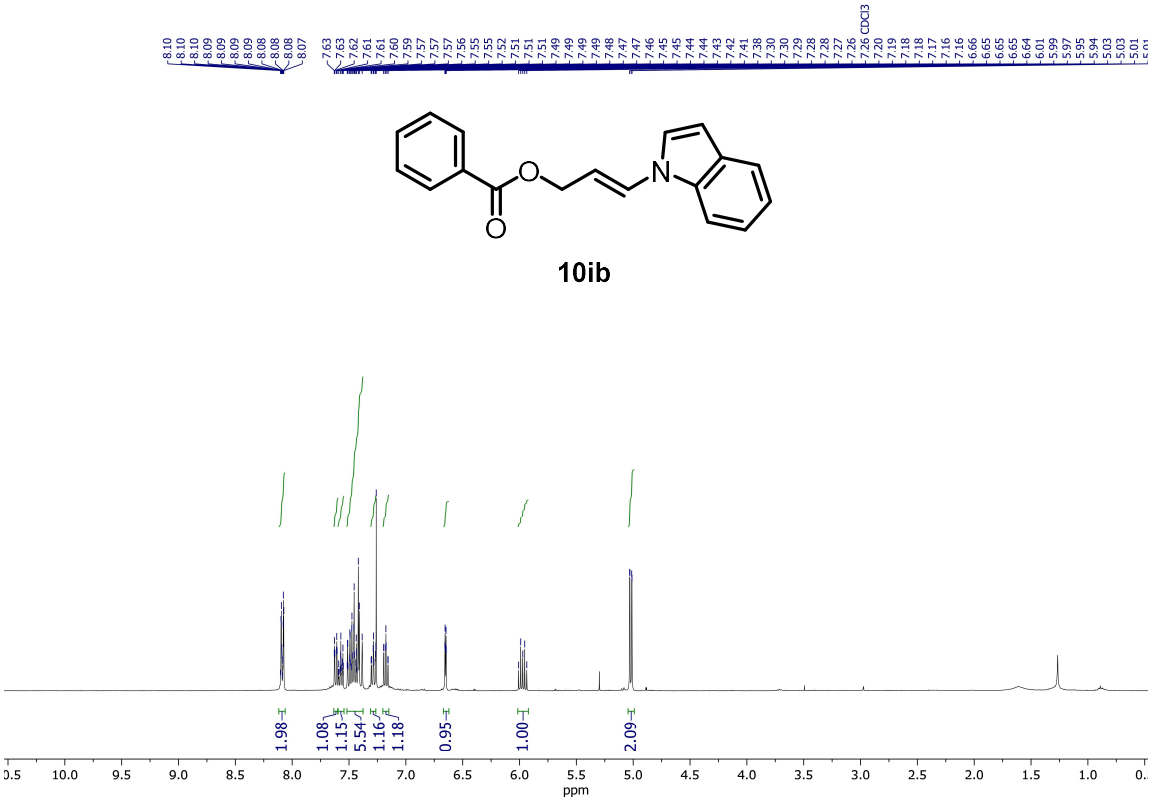
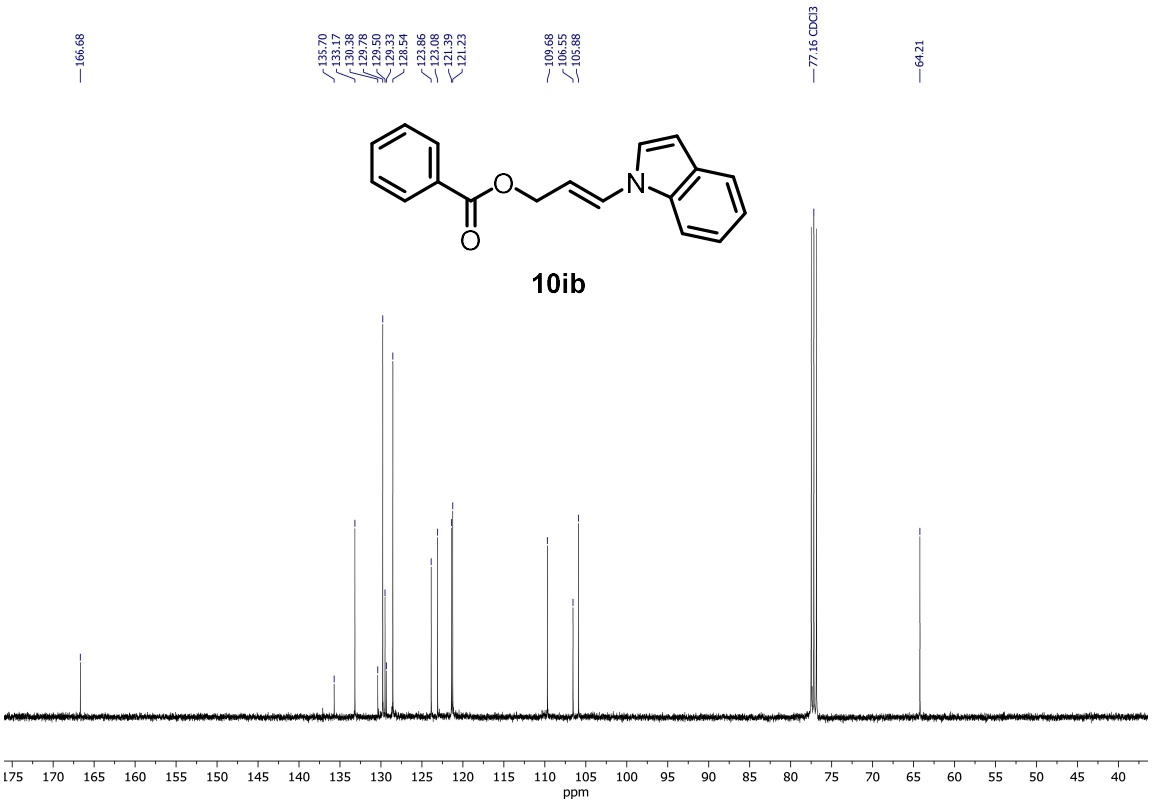


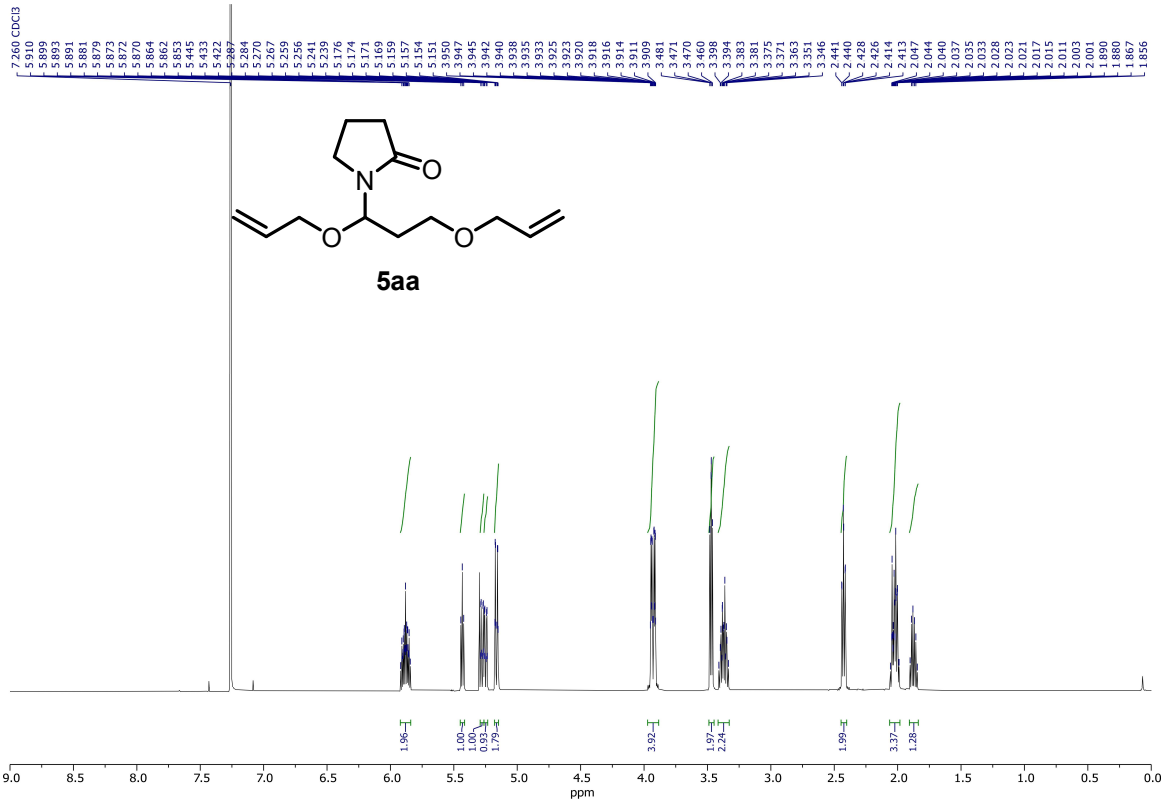
^{1}H NMR (400 MHz, $CDCl_3$)



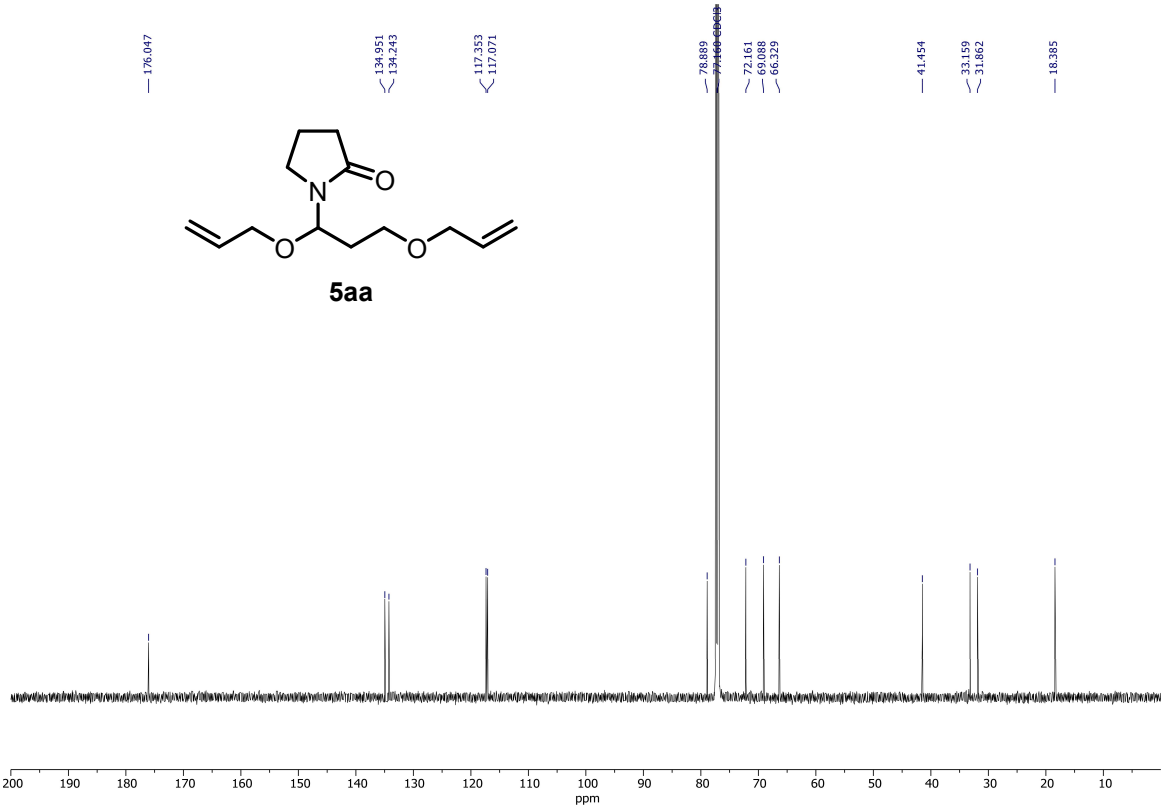
^{13}C NMR (100 MHz, $CDCl_3$)



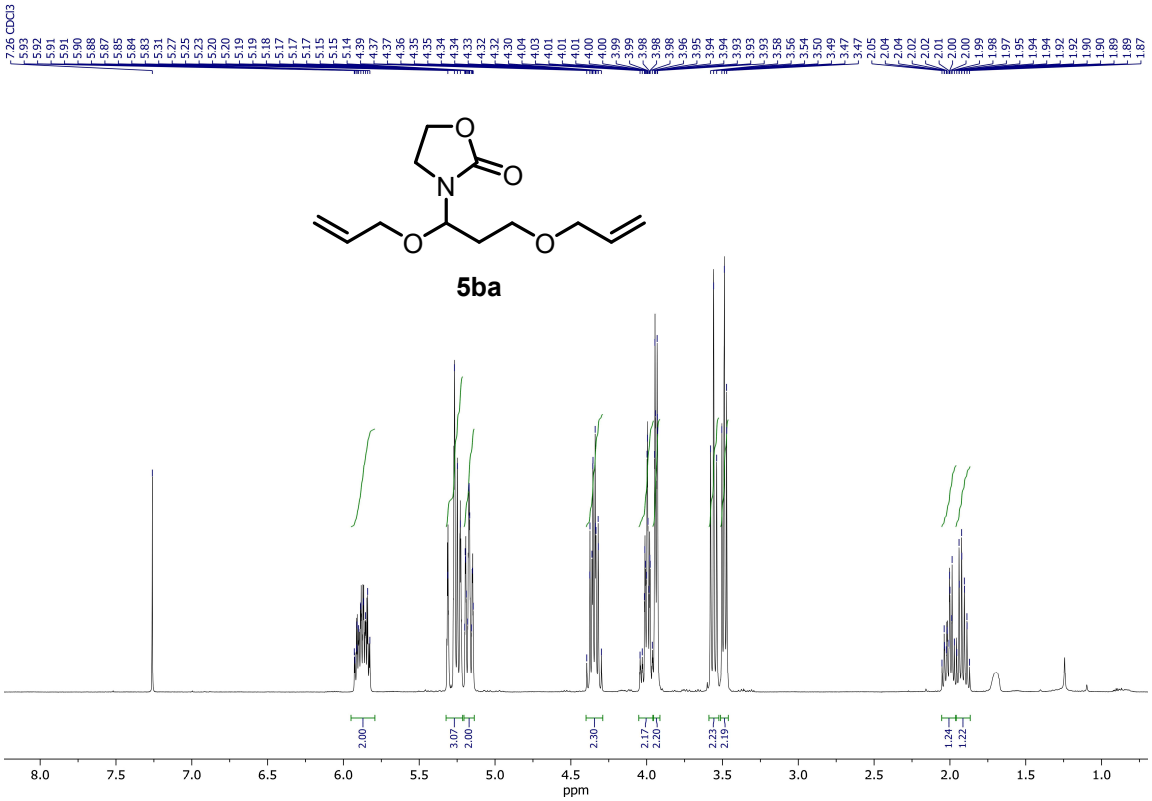
^{1}H NMR (600 MHz, $CDCl_3$)



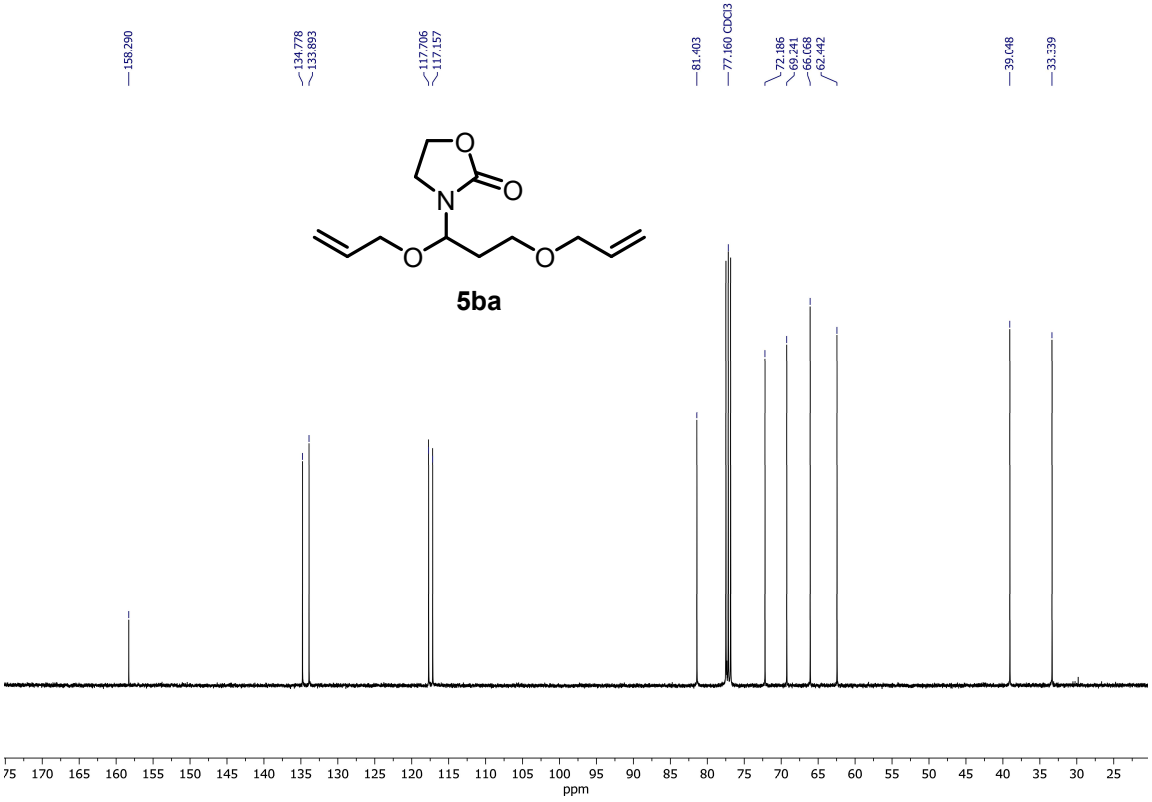
^{13}C NMR (100 MHz, $CDCl_3$)



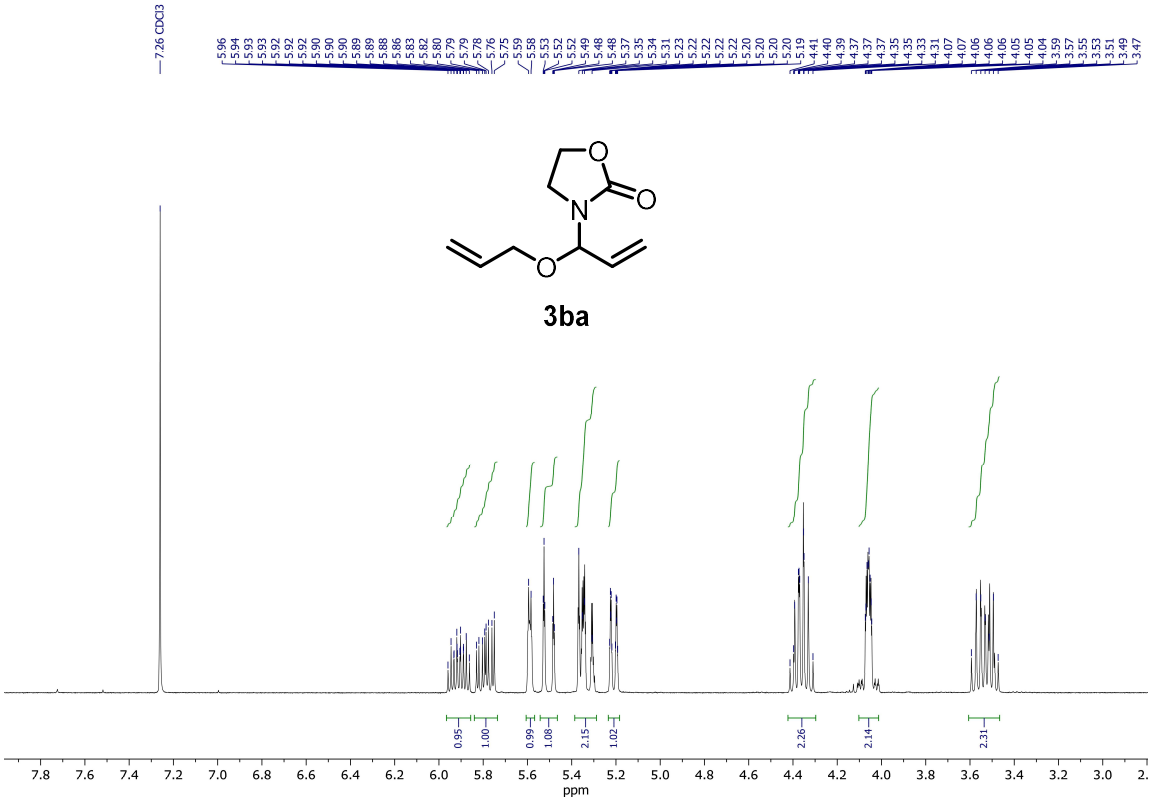
^{1}H NMR (400 MHz, $CDCl_3$)



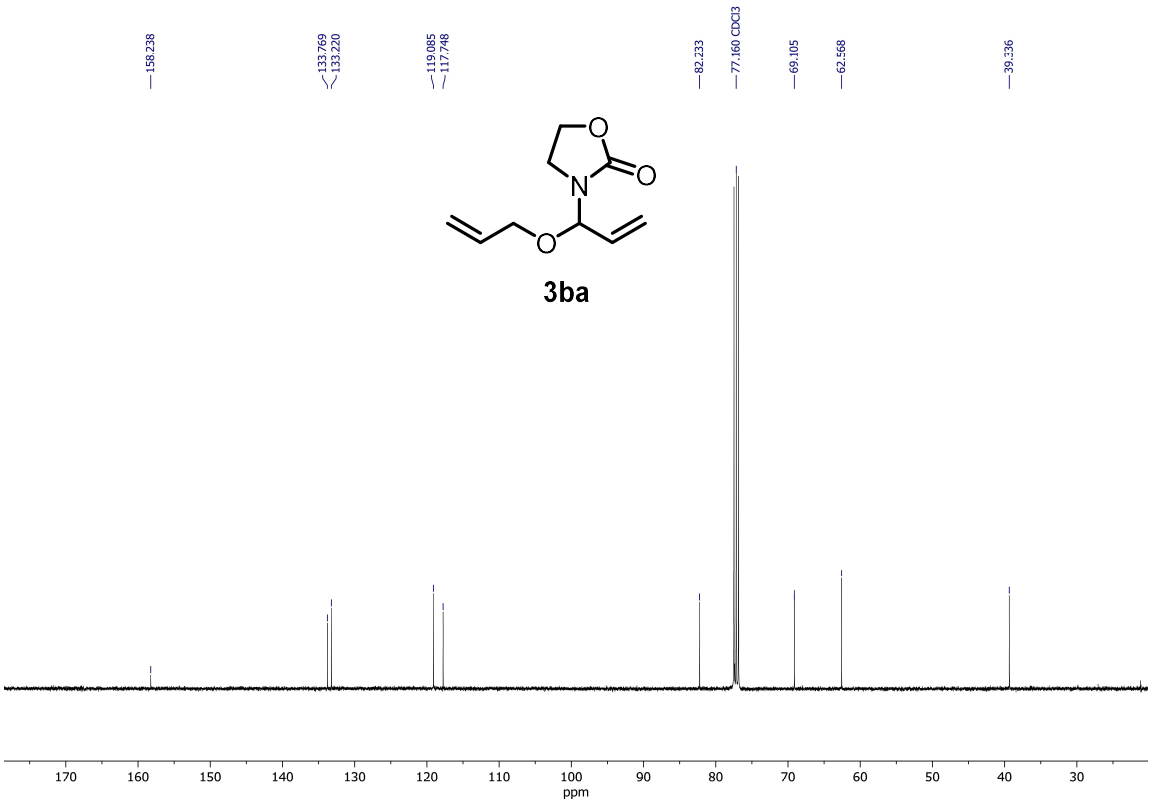
^{13}C NMR (100 MHz, $CDCl_3$)



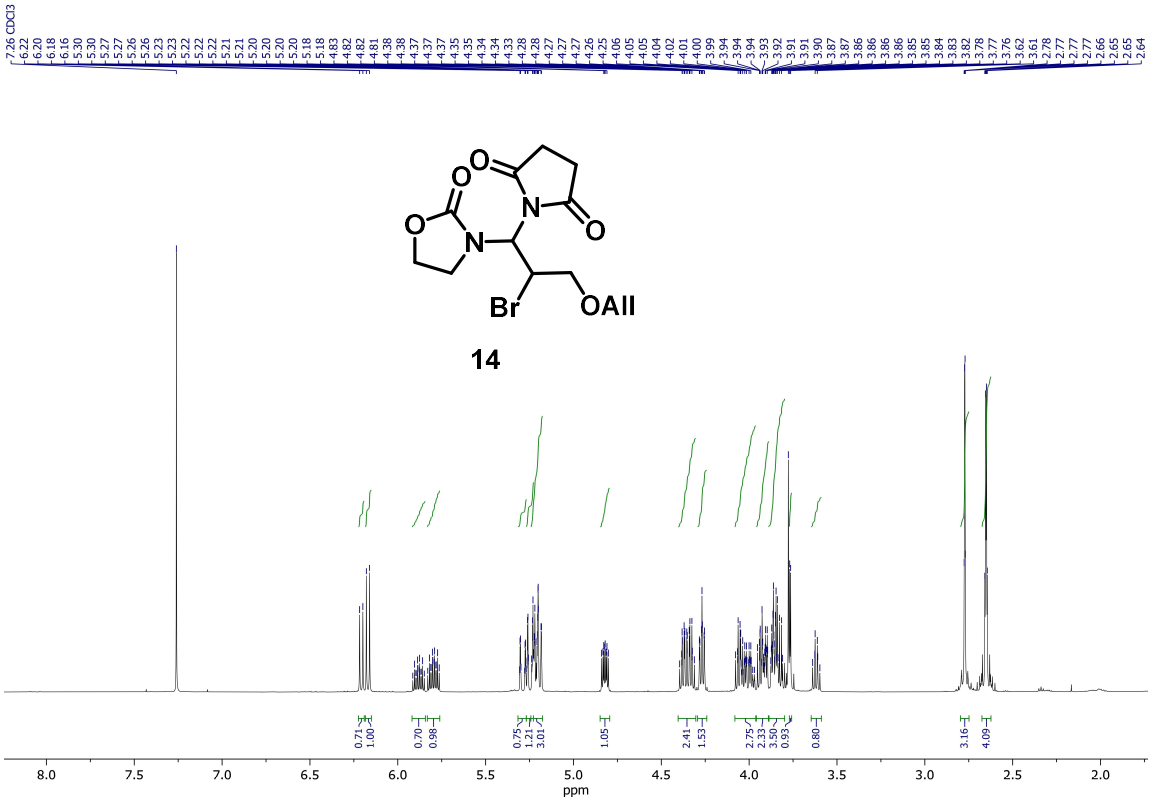
^{1}H NMR (400 MHz, $CDCl_3$)



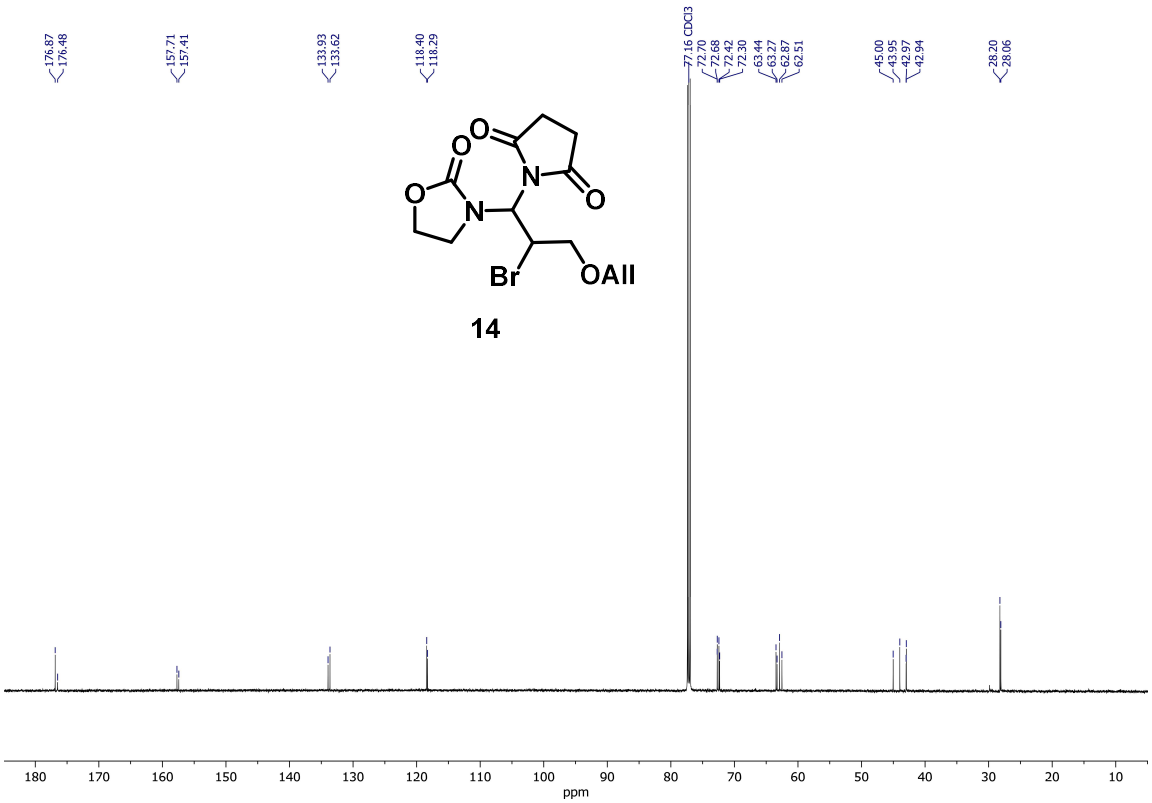
^{13}C NMR (100 MHz, $CDCl_3$)



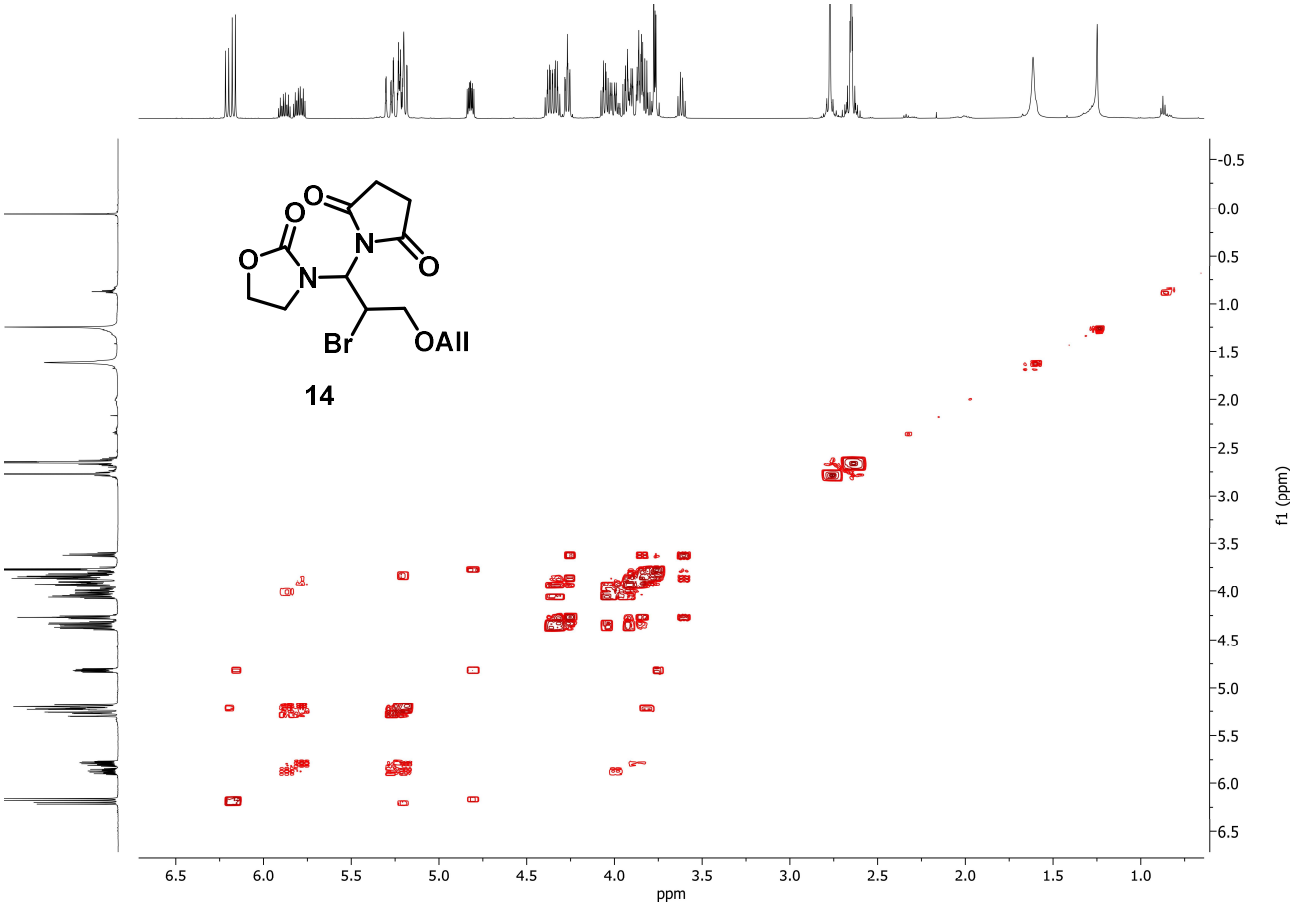
^{1}H NMR (600 MHz, $CDCl_3$)



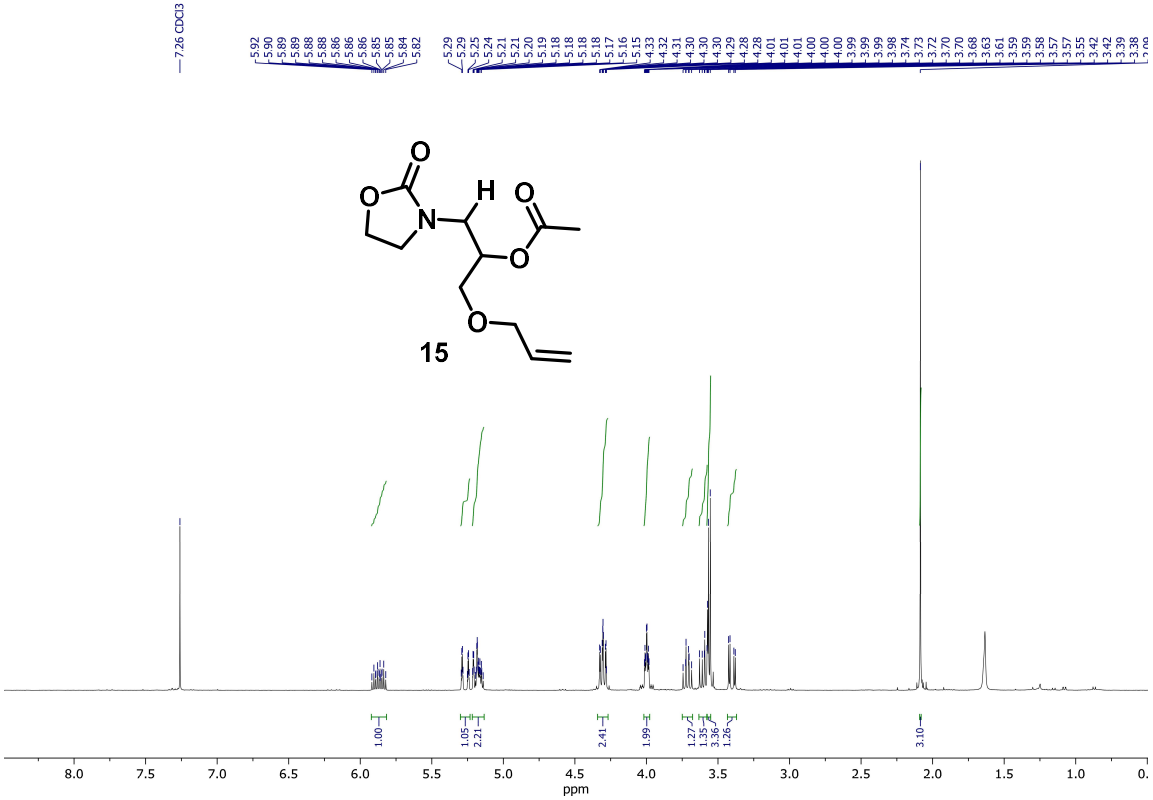
^{13}C NMR (150 MHz, $CDCl_3$)



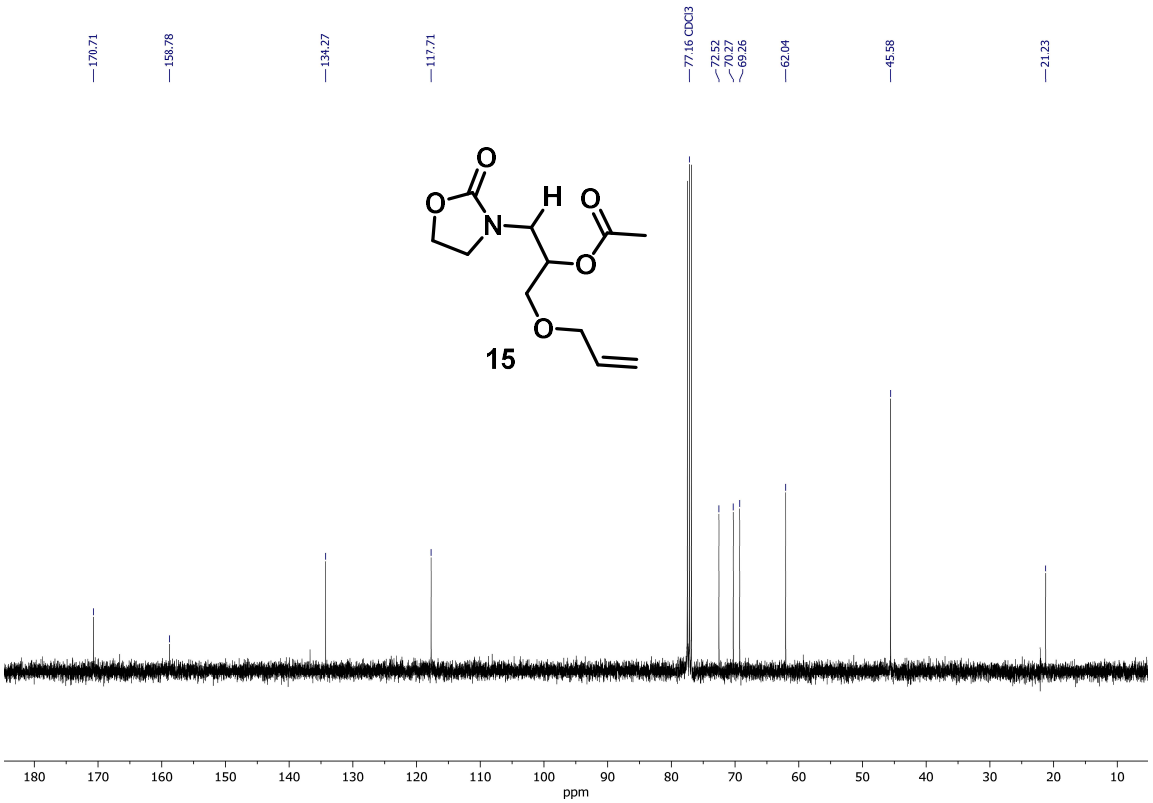
^{1}H – ^{1}H COSY


O
O
O
N
N
O
Br
OAll
14
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
f1 (ppm)
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

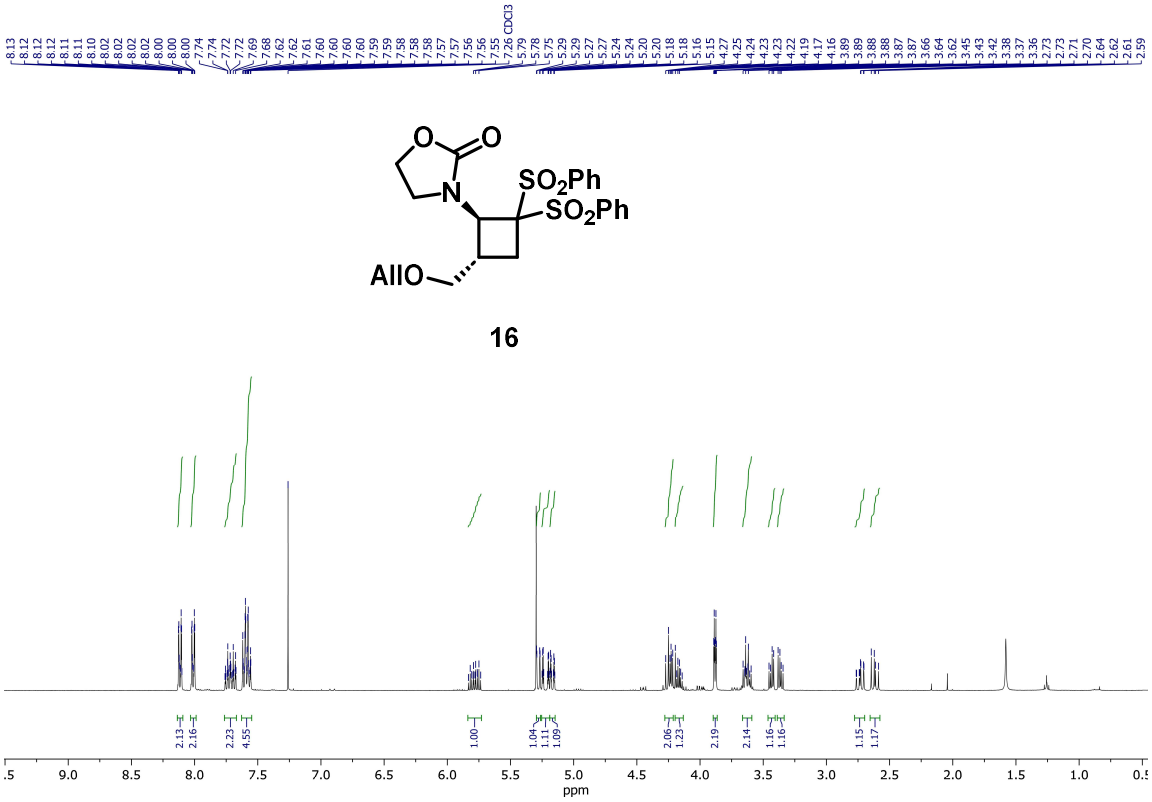
^{1}H NMR (400 MHz, $CDCl_3$)



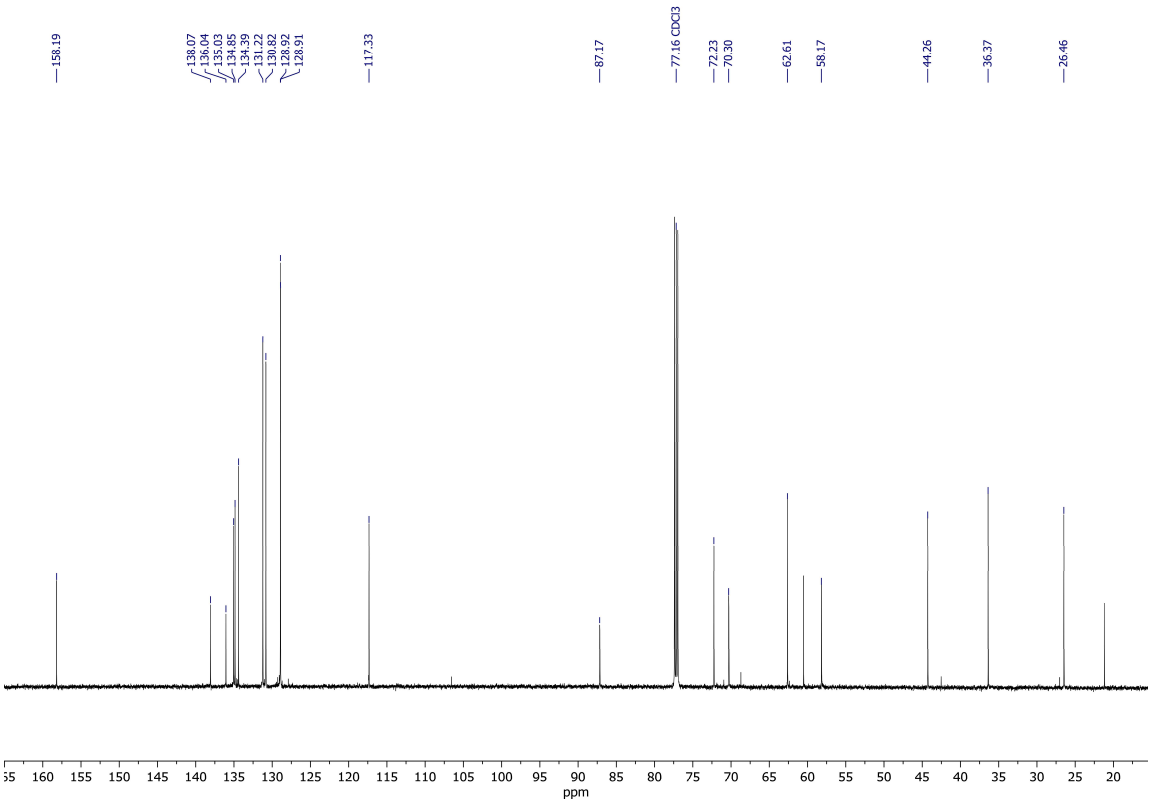
^{13}C NMR (100 MHz, $CDCl_3$)



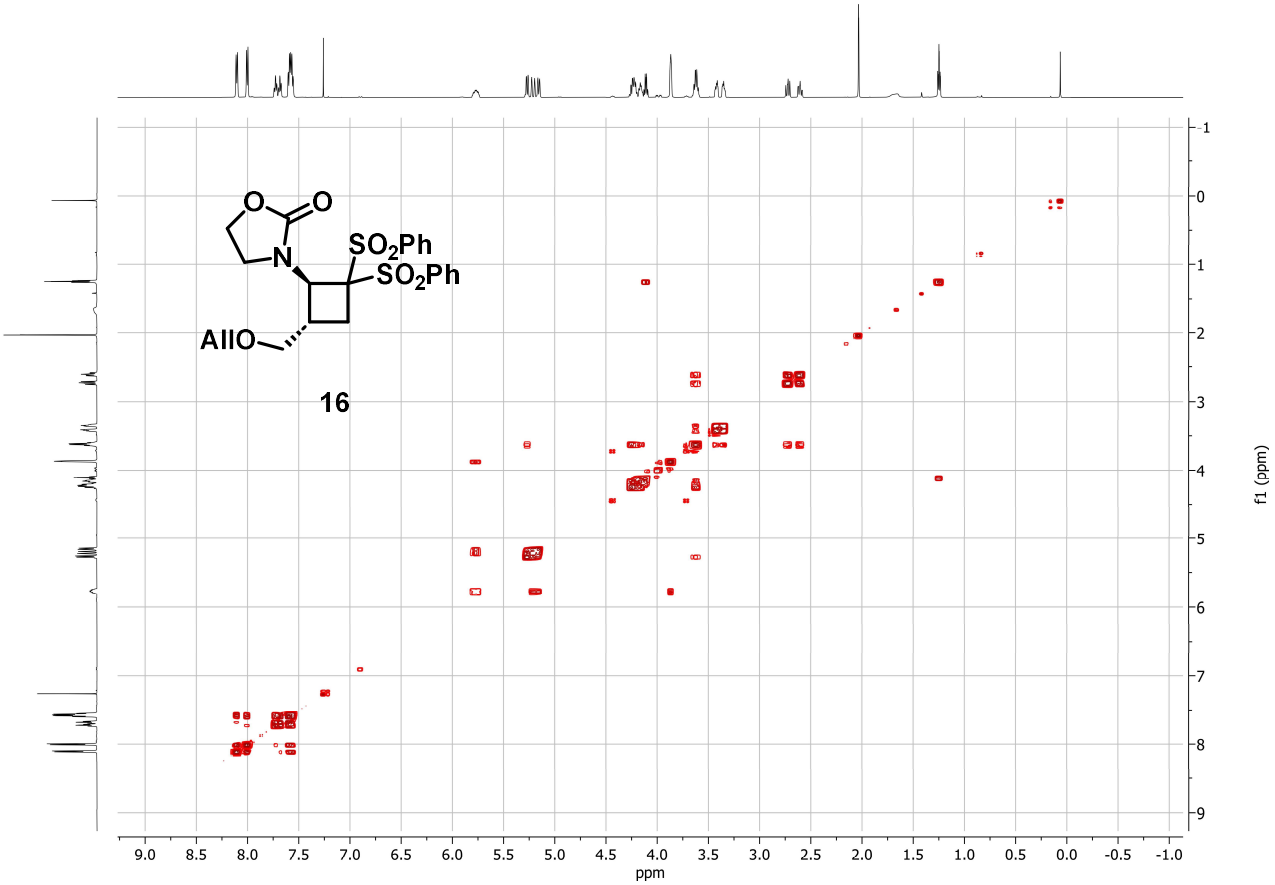
^{1}H NMR (600 MHz, $CDCl_3$)



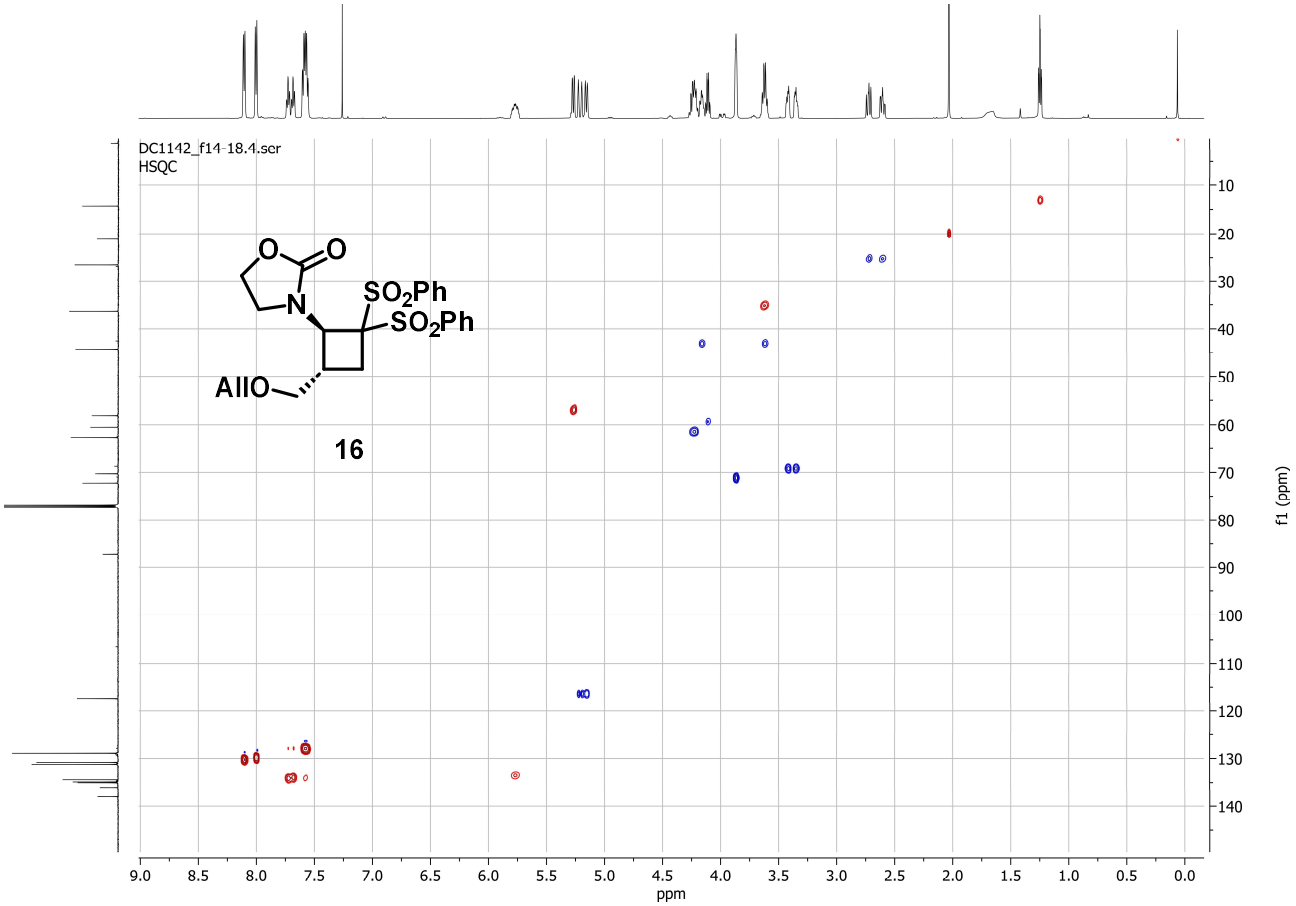
^{13}C NMR (150 MHz, $CDCl_3$)



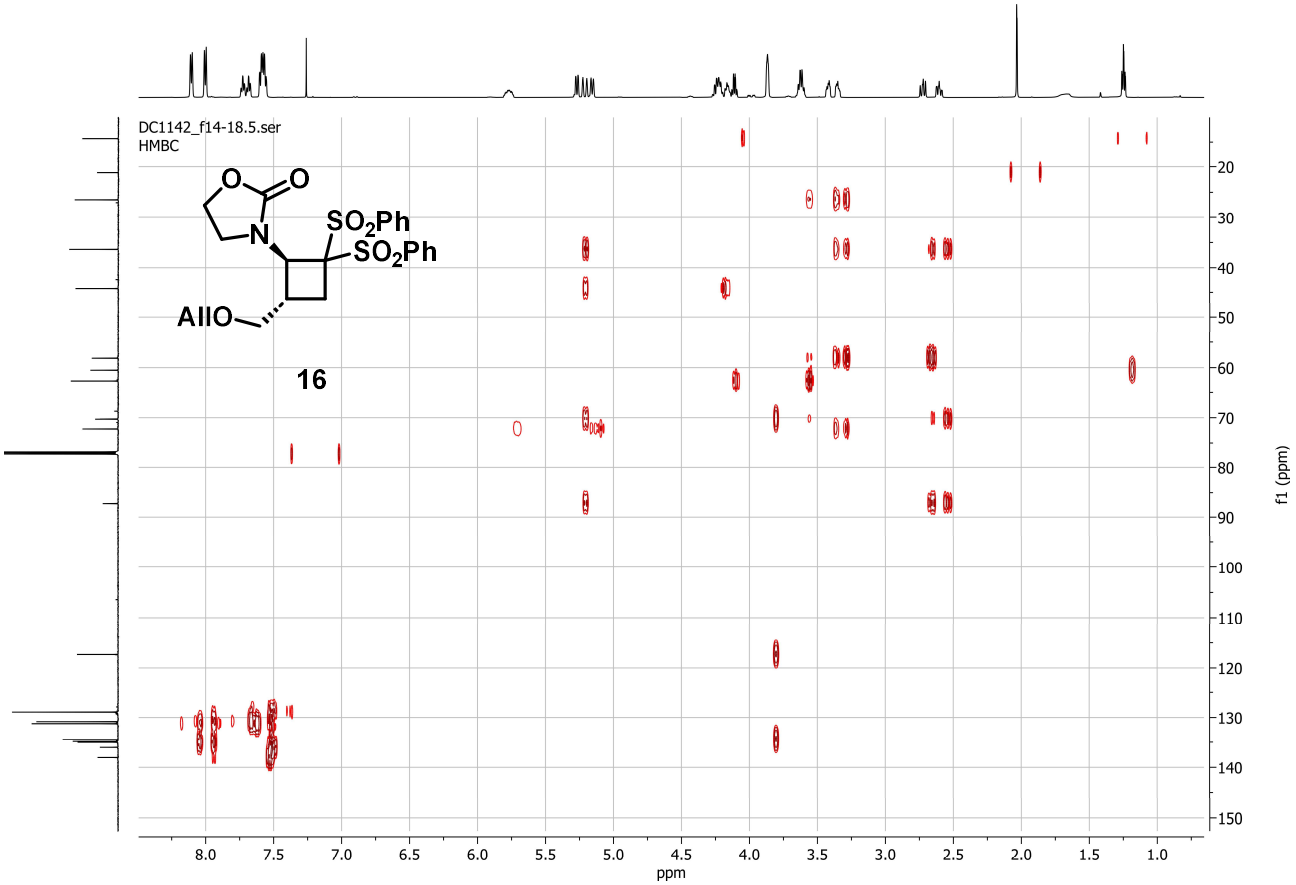
^{1}H – ^{1}H COSY



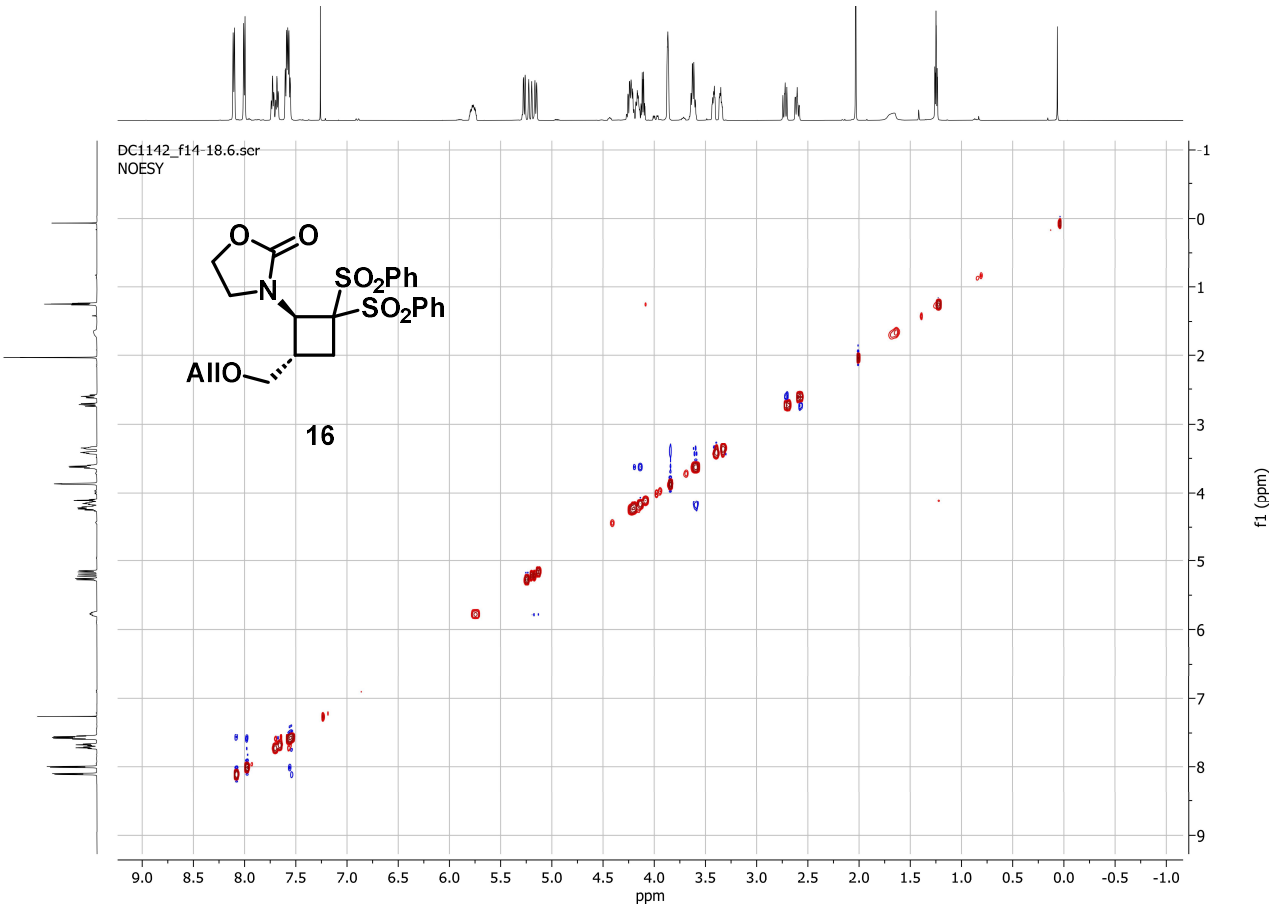
^{1}H – ^{13}C HSQC



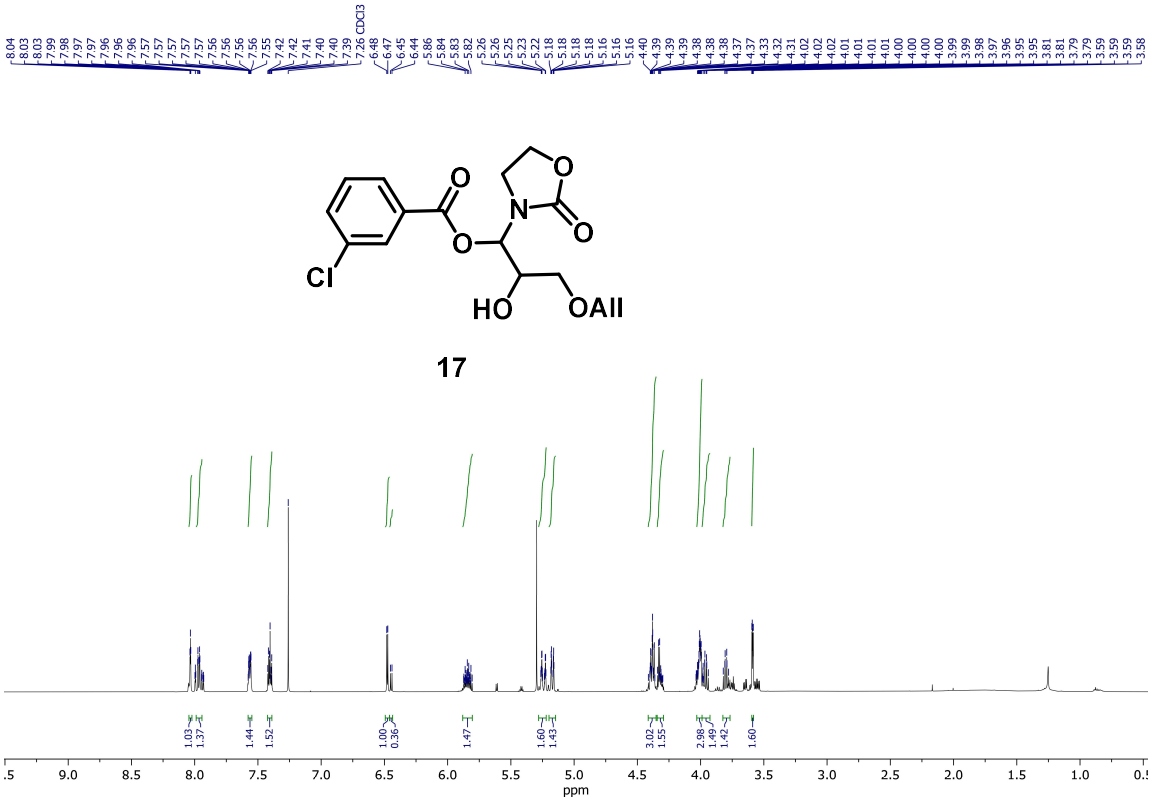
^{1}H – ^{13}C HMBC



2D NOESY



^{1}H NMR (600 MHz, $CDCl_3$)



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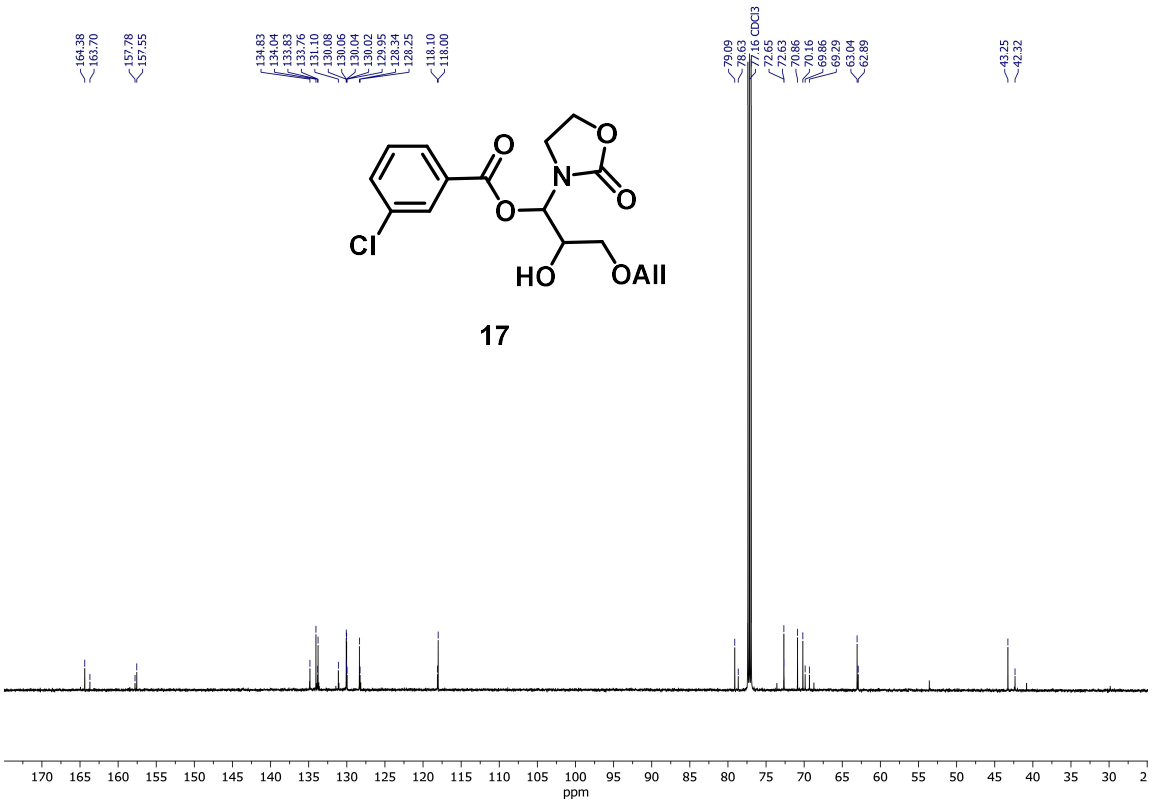
^{13}C NMR (150 MHz, $CDCl_3$)



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