Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Utilization of methanol for condensation interrupted chemoselective transfer hydrogenation of C=C, C=O, and C=N bonds under low catalyst loading

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1. General Consideration

1.1 Reagent Information : Unless otherwise stated, all the experiments were carried out under argon atmosphere using either argon filled Glove box or standard schlenk line technique. Glass apparatus were oven dried immediately prior to use. Solvents were dried according to the literature methods. Methanol was eventually distilled over sodium under argon atmosphere and deoxygenated prior to use. All the commercially available reagents were purchased from Sigma-Aldrich, Alfa-Aesar, TCI chemicals, SD-fine chemicals, Avra, Spectrochem. $IrCl_3.H_2O$ (99% extrapure) was purchased from SRL, India. For column chromatography, silica gel was used unless otherwise stated. A gradient elution using hexane/ethyl acetate or ethyl acetate/methanol was performed, based on silica TLC plate.

1.2 Analytical Information : ^{1}H and ^{13}C spectra were recorded on JEOL 400 MHz, and 500 MHz Spectrometer using $CDCl_3$, and DMSO-d_6. All ^{1}H NMR experiments were reported in parts per million (ppm) units and were measured relative to the signals for residual chloroform (7.24 ppm), and residual DMSO (2.5 ppm) in the deuterated solvent, unless otherwise stated and coupling constant (*J*) was reported in hertz (Hz). All ^{1}H decoupled ^{13}C NMR spectra were reported in ppm relative to deuterated chloroform (77.1 ppm), DMSO-d_6 (39.5). All the GC analysis were performed using Perkein Elmer Clarus 600 Gas Chromatograph and GC-MS were taken using Agilent 7890A Gas Chromatograph equipped with Agilent 5890 triple-quadrupole mass system.

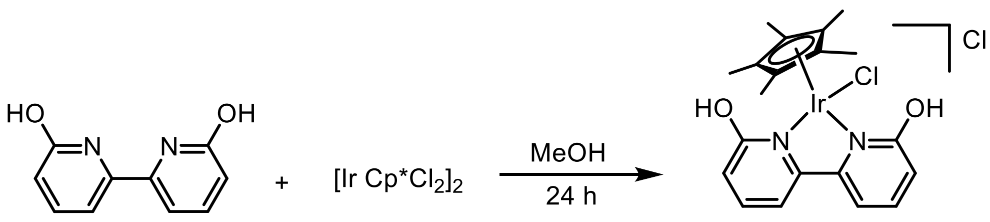
2. General Synthetic Procedures

2.1 Procedure for Synthesis of Ligands and Metal Complexes

All the ligands and their corresponding metal complexes were synthesized following the procedures reported in the literature.[1-3]

2.2 Procedure for Synthesis of Cat. 9[4]

Cat. **9** was synthesized by staring [1,1'-biphenyl]-3,3'-diol (186.2 mg, 1mmol) with [Ir Cp*Cl$_2$]$_2$ (398.4 mg, 0.5 mmol) in methanol at room temperature for 24 h. Synthesized complex was characterized by ^{1}H NMR, ^{13}C NMR, and ESI-MS analysis.



Cat. **9**, 85%

Scheme S1 Synthesis of Cat. **9**

2.2 Synthesis of α,β-Unsaturated Ketone Derivatives:[5]

An oven dried 25 mL round bottom flask (RB) was charged with a magnetic stir-bar, aryl ketone derivative (1.0 mmol), and aldehyde derivative (1.0 mmol), followed by the addition of ethanol (5.0 mL). Then 10% aqueous solution of NaOH (1.5 equiv.) was added dropwise in the stirring solution under ice cold condition. The stirring was continued for 5 h. After completion of the reaction, the reaction mixture was cooled in refrigerator overnight and yellowish white precipitate was obtained. Then the precipitate was collected through filtration, and washed with ice cold water-ethanol mixture until the pH of the filtrate becomes 7. Finally, the desired α, β-unsaturated ketone was purified through column chromatography (silica gel) using hexane-ethyl acetate as eluent. All the substrates were characterized by GC-MS analysis and ^1H NMR spectroscopy.

2.3 Transfer Hydrogenation of C=C, C=O and C=N bonds:

2.3.1 Optimization for Transfer Hydrogenation of C=C Bond in Chalcones:

An oven dried 4 mL screw cap tube was taken inside the argon filled glove box and charged with a magnetic stir-bar, chalcone **1a** (20.80 mg, 0.10 mmol), Cat. **6** (0.05 - 0.10 mol%), and $CsOH.H_2O$ (3-4 mol%), followed by the addition of methanol (0.7 mL). Then, the tube was sealed and placed in a preheated oil bath at 70-80 °C (oil bath temperature) for 3-4 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, 25 µL reaction mixture was syringed out and filtered through a small plug of silica and subjected for GC analysis using mesitylene as internal standard to determine conversion and yield of the product.

2.3.2 Synthesis of Saturated Ketones from α, β-Unsaturated Ketone Derivatives:

An oven dried 9 mL screw cap tube was taken inside the argon filled glove box and charged with a magnetic stir-bar, α,β-unsaturated ketone (**Xa**) (0.50 mmol), Cat. **6** (0.10 - 0.20 mol%), and CsOH. H_2O (4-8 mol%), followed by the addition of methanol (3.5 mL). Then, the tube was sealed and placed in a preheated oil bath at 80 °C (oil bath temperature) for 4 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the solvent was evaporated and the crude residue was purified by silica gel column chromatography using hexane-ethyl acetate as eluent which afforded the desired product.

2.3.3 Optimization for Double Transfer Hydrogenation of C=C and C=O Bonds in Chalcones:

An oven dried 4 mL screw cap tube was taken inside the argon filled glove box and charged with a magnetic stir-bar, chalcone **1a** (20.80 mg, 0.10 mmol), Cat. **6** (0.05 - 0.10 mol%), and base (4-20 mol%), followed by the addition of methanol (0.7 mL) or $MeOH/H_2O$ mixture. Then, the tube was sealed and placed in a preheated oil bath at 80-90 °C (oil bath temperature) for 3-12 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the reaction mixture was subjected for ^1H NMR analysis using 1,3,5-trimethoxybenzene as internal standard to determine conversion and yield of the product.

2.3.4 Synthesis of Alcohols from α, β-Unsaturated Ketone Derivatives:

An oven dried 9 mL screw cap tube was taken inside the argon filled glove box and charged with a magnetic stir-bar, α,β-unsaturated ketone (**Xa**) (0.50 mmol), Cat. **6** (0.50 mol%), and NaOAc (20 mol%), followed by the addition of $MeOH/H_2O$ in 13:1 ratio (3.5 mL). Then, the tube was sealed and placed in a preheated oil bath at 90 °C (oil bath temperature) for 12 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the solvent was evaporated, and the crude residue was purified by silica gel column chromatography using hexane-ethyl acetate as eluent which afforded the desired product.

2.3.5 Optimization for Transfer Hydrogenation of Imines:

An oven dried 4 mL screw cap tube was taken inside the argon filled glove box and charged with a magnetic stir-bar, N-benzyl-1-phenylmethanimine **59a** (19.50 mg, 0.10 mmol), Cat. **6** (0.10 - 0.30 mol%), and Cs_2CO_3 (4-6 mol%), followed by the addition of methanol (0.7 mL). Then, the tube was sealed and placed in a preheated oil bath at 80 °C (oil bath temperature) for 3 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the reaction mixture was evaporated and subjected for ^{1}H NMR analysis using 1,3,5-trimethoxy benzene as internal standard to determine conversion.

2.3.6 Synthesis of Secondary Amines:

An oven dried 9 mL screw cap tube was taken inside the argon filled glove box and charged with a magnetic stir-bar, Imine (**Xa**) (0.50 mmol), Cat. **6** (0.30 - 0.50 mol%), and Cs_2CO_3 (6-8 mol%), followed by the addition of methanol (3.5 mL). Then, the tube was sealed and placed in a preheated oil bath at 80 °C (oil bath temperature) for 3 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the solvent was evaporated, and the crude residue was purified by alumina column chromatography using hexane-ethyl acetate as eluent which afforded the desired product.

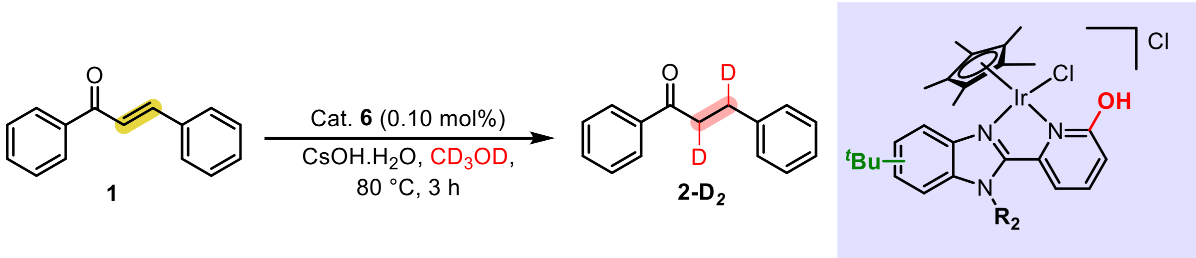
3. Preparative Scale Synthesis

An oven dried 60 mL screw cap tube was taken inside the argon filled glove box and charged with a magnetic stir-bar, α,β-unsaturated ketone/ imine (1.0 g), Cat. **6** (0.10-0.30 mol%), $CsOH.H_2O$/ NaOAc/Cs_2CO_3 (4-20 mol%) followed by the addition of methanol or MeOH/H_2O in 13:1 ratio (20.0 mL). Then the tube was sealed and placed in a preheated oil bath at 80-90 °C (oil bath temperature) for 3-12 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the solvent was evaporated and the crude residue was purified by silica gel/ alumina column chromatography using hexane-ethyl acetate as eluent which afforded the desired product.

4. Control Experiments

4.1 Deuterium Labelling Experiment:

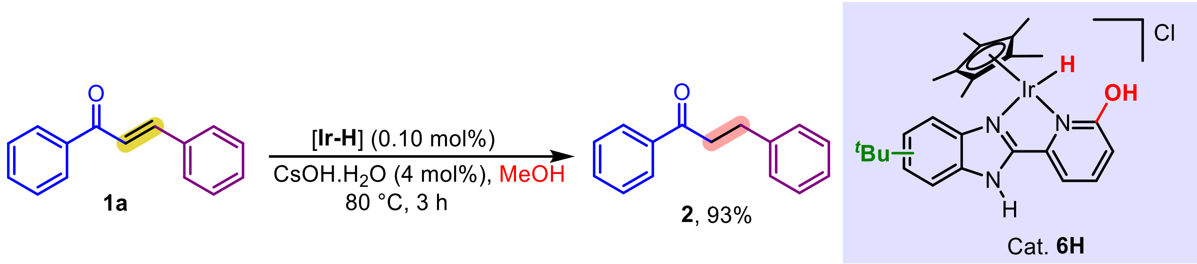
An oven dried 4 mL screw cap tube was taken inside the argon filled glove box and charged with a magnetic stir-bar, chalcone **1a** (20.80 mg, 0.10 mmol), Cat. **1** (0.05 mol%), and $CsOH.H_2O$ (4 mol%), followed by the addition of methanol (0.7 mL). Then, the tube was sealed and placed in a preheated oil bath at 80 °C (oil bath temperature) for 3 h. After completion of the reaction, the tube was allowed to cool at room temperature and the solvent was evaporated under reduced pressure. An appropriate amount of internal standard (mesitylene) was added to the reaction mixture. The yield of the methylated product, **2** was found to be 56% though GC analysis. The deuterium incorporated product **2-D₂** was confirmed from ESI-MS analysis. **ESI-MS:** Calcd for $C_{15}H_{12}D_2O$, $[M+H]^+$, 213.1248; found 213.1238. (Scheme S1).



Scheme S2 Deuterium labelling experiment

4.2 Synthesis and evaluation of reactivity for Ir(III)-H Species (Cat. 6H):

The Ir(III)-H (Cat. **6H**) was synthesized following the previous literature method.[3] The evaluation of its reactivity was performed under optimized reaction condition.



Scheme S3 Reactivity for Ir(III)-H species for TH of C=C bond of chalcone (**1**)

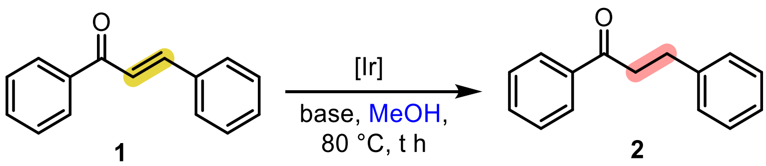
5. Kinetic Studies

5.1 Time Dependent Study:

A number of experiments for the synthesis of 1,3-diphenylpropan-1-one from chalcone (**1**) were conducted following the outlined procedure with varying time. An oven dried screw cap tube was charged with chalcone (**1**) (15 mg, 0.072 mmol), Cat. **6** (0.10 mol %), $CsOH.H_2O$ (4 mol%) followed by the addition of methanol (0.7 mL). All the tubes were placed in a preheated oil-baths at 80 °C with stirring. The progress of the reaction was monitored by gas chromatography using mesitylene as internal standard. All the reactions were repeated twice and the average data were plotted as conversion (%) vs time (min).

5.2 Determination of Reaction Order for Tandem Conversion of Chalcone to Saturated Ketone:

Two identical experiments were carried out following the general procedure varying only the amount of chalcone, **1**. After completion of the reaction, the tube was allowed to cool at room temperature and the mixture was filtered through a small plug of silica gel and directly subjected for GC analysis using mesitylene as internal standard to determine the yield of the saturated ketone, **2**. Accordingly, the concentration the final product was calculated at different time. All the reactions were repeated twice and the average data were plotted as product conc. vs time (min) in the Figure S1. Then, the initial rate for the different run was calculated to determine the order with respect to **1**.



Run	Chalcone (**1a**) (mmol)	Cat. **6** (10^{-4} mmol)	Base (10^{-3} mmol)	Methanol (mmol)
1	0.10 mmol	1	4	1 mL
2	0.20 mmol	0.50	2	1 mL

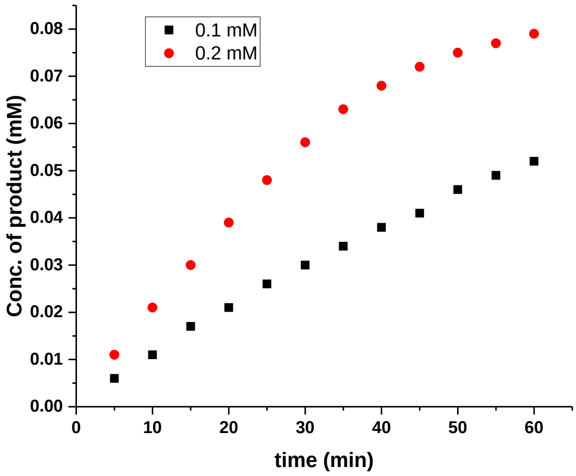


Figure S1 Determination of initial slopes for the TH of C=C bond of chalcone (**1**).

Considering steady state approximation for methanol

$$\text{Initial slope for run 1 at 60 min } (r_1) = 9.1190 \times 10^{-4} \text{ (mM)/min} = k\,[1a\ (0.10\ \text{mmol})]^x$$

$$\text{Initial slope for run 2 at 60 min } (r_2) = 16.5714 \times 10^{-4} \text{ (mM)/min} = k\,[1a\ (0.20\ \text{mmol})]^x$$

$$\text{Comparing the initial slopes, } r_1/r_2 = 16.5714/9.1190 = (0.20/0.10)^x$$

$$\text{or, } 1.820 = (2.0)^x$$

$$\text{or, } \log(1.820) = \log(2.0)^x$$

$$\text{or, } x = \log(1.820)/\log(2.0)$$

$$\text{or, } x = 0.864 \approx 1$$

$$\text{So, rate} = k[1a]^1$$

This experiment stated that C=C bond TH of chalcone (**1**) follow a first order kinetics with respect to the **1** concentration.

5.3 Kinetic Isotope Effect (KIE) Studies:

Parallel reactions for the synthesis of 1,3-diphenylpropan-1-one from chalcone (**1a**) were carried out using CH_3OH and CD_3OD under identical conditions following the outlined procedure. All the tubes were placed in a preheated oil-baths at 80 °C with stirring and the progress of the reaction was analysed by GC using mesitylene as internal standard. All the reactions were repeated twice and the average data were plotted as ln(a/a-x) vs time (min) (Figure S2)

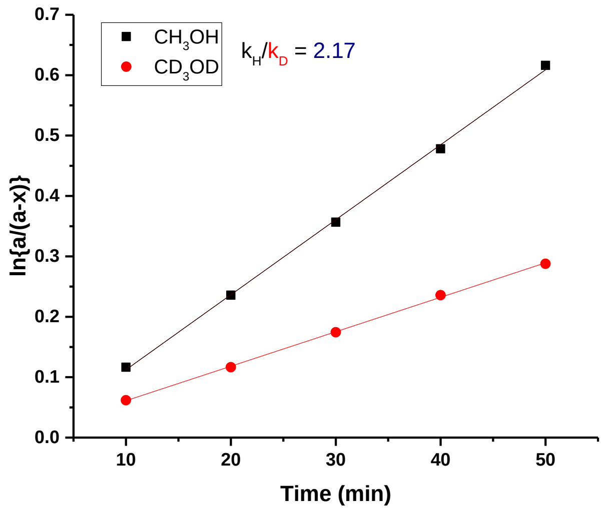
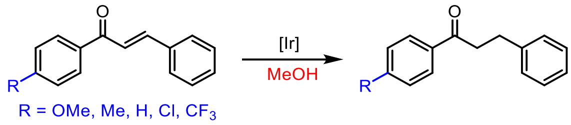


Figure S2 KIE study for TH of C=C bond of chalcone (**1**).

6. Hammett Studies:

An oven dried screw cap tube was charged with several electronically disparate chalcone derivatives (0.10 mmol), Cat. **1** (0.10 mol %), $CsOH.H_2O$ (4 mol%) followed by the addition of methanol. All the tubes were placed in a preheated oil-baths at 80 °C with stirring. The progress of the reaction was analysed by GC using mesitylene as internal standard. Reactivity towards the conversion of chalcone derivatives to saturated ketone compounds followed the sequence: 4-CF_3 >4-Cl>4-H >4-Me >4-OMe (Figure S3, and S4; Table S1).

Table S1 Hammett Analysis with the Para Substitution Constant (σ)



Substrate	k x 10^{-4} (min^{-1})	k_X/k_H	Log(k_X/k_H)	σP	ρ
4-OMe	54.0	0.43478	-0.36173	-0.268	
4-Me	70.6	0.56844	-0.24532	-0.17	
4-H	124.2	1	0	0	**+1.20**
4-Cl	181.6	1.46216	0.16499	0.227	
4-CF_3	540.0	4.34783	0.63827	0.544	

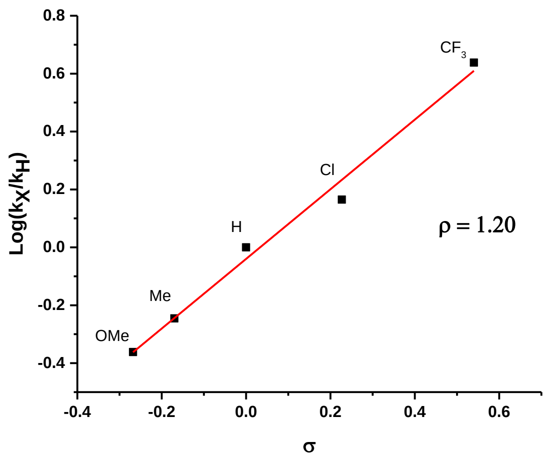


Figure S3 Hammett analysis using substitution constant σ- for conversion of chalcone derivatives to saturated ketone.

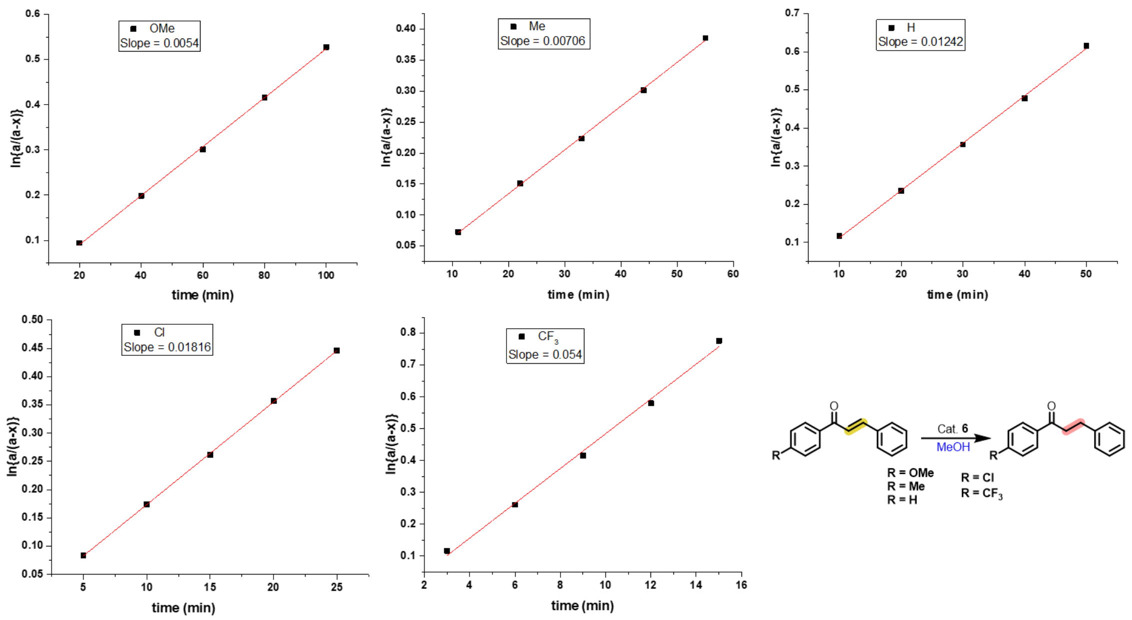


Figure S4 Determination of rate constant for the conversion of electronically disparate chalcones to saturated ketones.

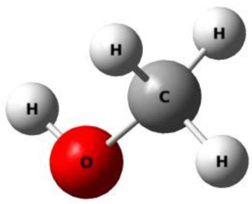
7. Transfer Hydrogenation of Nitro-substituted Chalcone (18a) at Different Time Duration:

An oven dried 4 mL screw cap tube was taken inside the argon filled glove box and charged with a magnetic stir-bar, chalcone **18a** (25.30 mg, 0.10 mmol), Cat. **6** (0.05 mol%), and NaOAc (20 mol%), followed by the addition of MeOH/H_2O mixture in 13:1 (v/v) ratio. Then, the tube was sealed and placed in a preheated oil bath at 90 °C (oil bath temperature) for 3-36 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the reaction mixture was subjected for ^{1}H NMR analysis using 1,3,5-trimethoxybenzene as internal standard to determine conversion and yield of the product.

8. Computational Studies:

All the calculations were performed using the Gaussian 09 package.[6] Full geometry optimization followed by frequency calculations on the stationary points were carried out to ascertain the nature of the stationary points as minima or first order saddle point. Hybrid functional, M06-2X was used with the LANL2DZ basis set[7] for Ir and 6-31G** basis set[8] for non-metal elements. The transition states (TS) were further confirmed by performing intrinsic reaction coordinate (IRC) calculation using the same method.

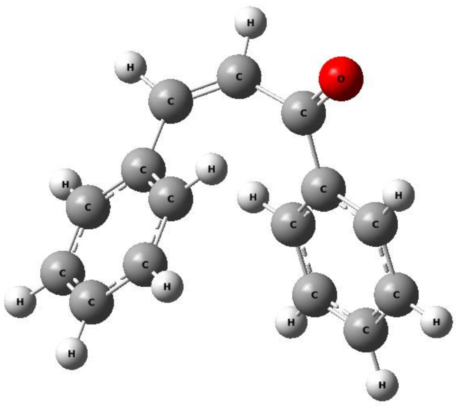
Methanol:



Methanol	
SCF Done: E (RM062X)	-115.632634
Thermal correction to Gibbs Free Energy	0.029621

C	0.67796500	-0.02077100	0.00000300
H	1.08039300	0.97990900	-0.00098900
H	1.03897300	-0.53855000	0.88256200
H	1.03884400	-0.54022600	-0.88162700
O	-0.75597400	0.12134300	0.00000300
H	-1.17820200	-0.74725200	0.00001000

Chalcone:

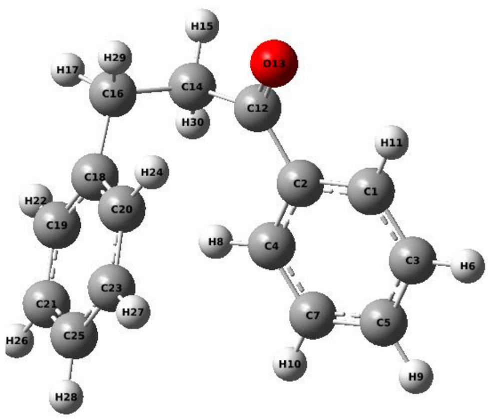


Chalcone	
SCF Done: E (RM062X)	-653.565828
Thermal correction to Gibbs Free Energy	0.185714

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38891257
C	1.18819352	0.00000000	-0.70113078

C	1.20986066	0.02544536	2.06721140
C	2.39320348	0.01607206	-0.01743113
H	1.17777185	-0.00904766	-1.77260087
C	2.40266063	0.03577576	1.36557320
H	1.23126673	0.06086980	3.13689517
H	3.31811713	0.01851935	-0.55935112
H	3.33289362	0.06287856	1.89686422
H	-0.94044223	0.00019305	-0.51033160
C	-1.33276810	0.01210953	2.07340486
O	-2.33027545	0.27651365	1.41921092
C	-1.34437637	-0.34503105	3.50464285
H	-0.53561217	-0.98736212	3.79270887
C	-2.19343571	-0.00490201	4.47232923
H	-1.94375059	-0.41587753	5.43599166
C	-3.37955417	0.87002525	4.55138557
C	-3.74177442	1.30171064	5.82977330
C	-4.16090282	1.26938897	3.46962043
C	-4.83189175	2.12415395	6.02427317
H	-3.15836278	0.99147519	6.67538775
C	-5.25784705	2.08828687	3.67006531
H	-3.90736478	0.93508379	2.49028589
C	-5.59534337	2.52109271	4.93927880
H	-5.08739928	2.44900674	7.01314371
H	-5.85143190	2.38439075	2.82806993
H	-6.44742441	3.15527229	5.08435150

1,3-diphenylpropan-1-one (2):

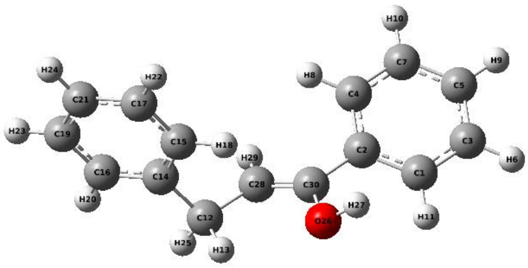


1,3-diphenylpropan-1-one	
SCF Done: E (RM062X)	**-654.770530**
Thermal correction to Gibbs Free Energy	**0.209978**

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38891257
C	1.18819352	0.00000000	-0.70113078
C	1.20986066	0.02544536	2.06721140
C	2.39320348	0.01607206	-0.01743113
H	1.17777185	-0.00904766	-1.77260087

C	2.40266063	0.03577576	1.36557320
H	1.23126673	0.06086980	3.13689517
H	3.31811713	0.01851935	-0.55935112
H	3.33289362	0.06287856	1.89686422
H	-0.94044223	0.00019305	-0.51033160
C	-1.33276810	0.01210953	2.07340486
O	-2.33027545	0.27651365	1.41921092
C	-1.34437637	-0.34503105	3.50464285
H	-0.53561217	-0.98736212	3.79270887
C	-2.19343571	-0.00490201	4.47232923
H	-1.94375059	-0.41587753	5.43599166
C	-3.37955417	0.87002525	4.55138557
C	-3.74177442	1.30171064	5.82977330
C	-4.16090282	1.26938897	3.46962043
C	-4.83189175	2.12415395	6.02427317
H	-3.15836278	0.99147519	6.67538775
C	-5.25784705	2.08828687	3.67006531
H	-3.90736478	0.93508379	2.49028589
C	-5.59534337	2.52109271	4.93927880
H	-5.08739928	2.44900674	7.01314371
H	-5.85143190	2.38439075	2.82806993
H	-6.44742441	3.15527229	5.08435150

1,3-diphenylprop-1-en-1-ol :

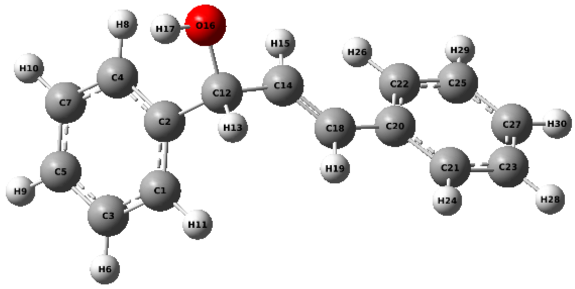


1,3-diphenylpropan-1-one	
SCF Done: E (RM062X)	-654.752225
Thermal correction to Gibbs Free Energy	0.207616

C	3.40317800	-0.81660300	0.31745300
C	2.21936800	-0.16734400	-0.05235000
C	4.61855100	-0.13977800	0.29577700
C	2.27682900	1.17870900	-0.43125000
C	4.66742300	1.19542800	-0.09355500
H	5.52916700	-0.65945400	0.57619800
C	3.49244900	1.85097000	-0.45807500
H	1.35717000	1.69869700	-0.68057000
H	5.61415300	1.72540900	-0.10898300
H	3.52187600	2.89595300	-0.74999500
H	3.37278100	-1.86733900	0.59243100
C	-1.39517000	-1.41039600	-0.80403600
H	-1.30330300	-2.26304500	-0.12478600

C	-2.49930700	-0.49239900	-0.31491300
C	-2.39610100	0.09003600	0.95196400
C	-3.61688700	-0.20382500	-1.09606900
C	-3.39062600	0.93451100	1.42929200
H	-1.52171000	-0.13247600	1.55911200
C	-4.61551700	0.64647600	-0.62294500
H	-3.70816000	-0.64972600	-2.08330800
C	-4.50529900	1.21747400	0.64035300
H	-3.29791700	1.37555500	2.41705600
H	-5.47915900	0.86308200	-1.24421800

1,3-diphenylprop-2-en-1-ol:



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SCF Done: E (RM062X)	-651.131554
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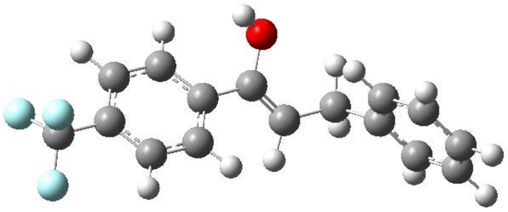
C	2.30693900	0.30664300	-0.26746300
C	3.25832700	-1.84358900	-0.82700900
C	3.14364800	0.38669300	0.84462600
C	4.10303700	-1.76020100	0.28351700
H	3.29928500	-2.71078600	-1.47527300
C	4.04183000	-0.64541700	1.12007600
H	3.07088300	1.26126600	1.47935500
H	4.80081500	-2.56136500	0.49467800
H	4.69094500	-0.58096700	1.98545500
H	1.69584300	-0.87835300	-1.95498100
C	1.31286500	1.43084500	-0.53310800
H	1.23121000	1.60050600	-1.61684000
C	-0.02609100	1.02889400	0.02463400
H	-0.08101800	1.08397900	1.10803300
O	1.70018900	2.63679000	0.18382800
H	2.57867600	2.93106300	-0.17499400
C	-1.03558100	0.59603200	-0.73101700
H	-0.91629800	0.59322200	-1.81409600
C	-2.34905100	0.12182600	-0.24994800
C	-3.37712000	-0.09048900	-1.18068200
C	-2.61278300	-0.12365600	1.10724700
C	-4.63694000	-0.52369200	-0.77045900
H	-3.18289500	0.09103800	-2.23260200
C	-3.87112000	-0.55421000	1.51783300
H	-1.82731300	0.01219600	1.84152500
C	-4.88929300	-0.75467100	0.58170200

H	-5.41867700	-0.67936100	-1.50450400
H	-4.05890300	-0.73964800	2.56862900
H	-5.86630600	-1.09231000	0.90495800

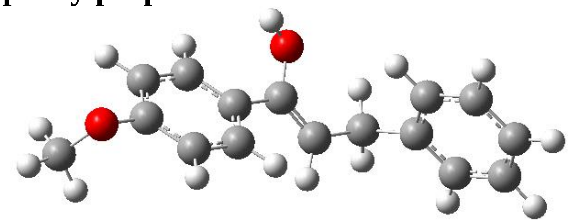
3-phenyl-1-(4-(trifluoromethyl)phenyl)prop-1-en-1-ol:



3-phenyl-1-(4-(trifluoromethyl)phenyl)prop-1-en-1-ol	
SCF Done: E (RM062X)	-991.682194
Thermal correction to Gibbs Free Energy	0.210503

C	-1.74123300	1.61792300	0.32065400
C	-0.68740500	0.76913300	-0.03809600
C	-3.05350100	1.15570800	0.32271100
C	-0.97462100	-0.55686200	-0.38156300
C	-3.33052000	-0.16130800	-0.03151000
H	-3.86075400	1.82847100	0.59410400
C	-2.28641100	-1.01466500	-0.38477100
H	-0.15821700	-1.23068800	-0.62190400
H	-2.49440200	-2.04658400	-0.64926000
H	-1.53147400	2.65492700	0.56805300
C	3.07781800	1.36499400	-0.84005700
H	3.13744100	2.23748200	-0.18275900
C	4.01582600	0.28615200	-0.33279100
C	3.82771600	-0.23891100	0.94931000
C	5.06136300	-0.20625700	-1.11179600
C	4.66997800	-1.22709400	1.44342600
H	3.00910200	0.14302800	1.55486200
C	5.90664900	-1.20097800	-0.62175300
H	5.21729800	0.19322200	-2.11074600
C	5.71352400	-1.71367600	0.65650800
H	4.51345100	-1.62153100	2.44278100
H	6.71553200	-1.57563300	-1.24152400
H	6.37025100	-2.48836100	1.03919300
H	3.39961700	1.68502700	-1.83707100
O	0.98028000	2.25613900	0.89169100
H	0.36960800	2.16026100	1.63173000
C	1.65408700	0.88461800	-0.88681500
H	1.38365800	0.16231100	-1.65018200
C	0.70355400	1.27824800	-0.03223400
C	-4.78191900	-0.67610900	-0.02706700
F	-5.06179600	-1.22281400	1.17513300
F	-5.62481700	0.35213500	-0.26102300
F	-4.93147300	-1.60893600	-0.99141500

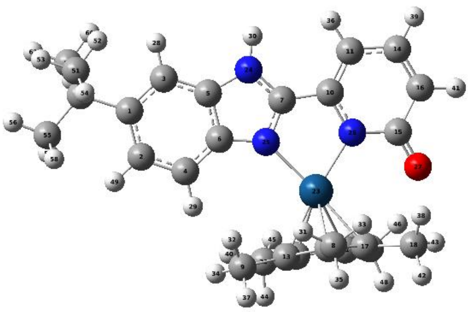
1-(4-methoxyphenyl)-3-phenylprop-1-en-1-ol:



1-(4-methoxyphenyl)-3-phenylprop-1-en-1-ol	
SCF Done: E (RM062X)	-769.191716
Thermal correction to Gibbs Free Energy	0.237529

C	2.47229200	1.31444900	-0.39338700
C	1.37374400	0.51479800	-0.05656900
C	3.74593800	0.76315900	-0.49135900
C	1.57589800	-0.85196700	0.16661800
C	3.93901100	-0.59485700	-0.25628800
H	4.58924100	1.39786400	-0.74416400
C	2.84959700	-1.39927600	0.07426300
H	0.72218300	-1.48451300	0.38882800
H	2.99133500	-2.46160200	0.24585700
H	2.32983500	2.38053800	-0.54747800
C	-2.30323800	1.30455800	0.95890200
H	-2.32420300	2.23056400	0.37674700
C	-3.33714100	0.33989600	0.40976700
C	-3.23841500	-0.08895100	-0.91733700
C	-4.38479500	-0.14090500	1.19316700
C	-4.16972500	-0.97129100	-1.45043900
H	-2.41823800	0.28355900	-1.52663500
C	-5.31944000	-1.02987000	0.66373300
H	-4.47176200	0.18432000	2.22683300
C	-5.21465700	-1.44709500	-0.65878400
H	-4.08181400	-1.29151200	-2.48413300
H	-6.12882900	-1.39699900	1.28733600
H	-5.94102300	-2.13944200	-1.07221300
H	-2.56141000	1.56259400	1.99175200
O	-0.21517000	2.18699300	-0.78867800
H	0.35740000	2.11023500	-1.56071600
C	-0.91794400	0.72335300	0.90307800
H	-0.67171600	-0.07692900	1.59337400
C	0.02481900	1.11888400	0.04080200
O	5.24674900	-1.16418500	-0.35917700
C	6.02226900	-0.78799300	0.78185300
H	6.92761500	-1.35796400	0.80142900
H	6.25806000	0.25415400	0.72499700
H	5.46141700	-0.97868400	1.67290900

I$_0$

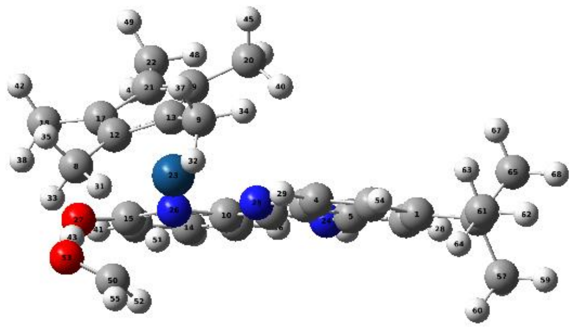


I$_0$	
SCF Done: E (RM062X)	**-1352.406182**
Thermal correction to Gibbs Free Energy	**0.463352**

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.41236210
C	1.22217618	0.00000000	-0.67253812
C	1.16349657	0.01417541	2.16749111
C	2.38522615	0.01364470	0.08631692
C	2.37850016	0.03722865	1.48982562
C	4.46554468	-0.01181733	0.84388573
C	4.67969762	3.15353651	5.00183505
C	2.01730864	1.49133680	5.16658595
C	5.90688315	-0.10627639	1.00719166
C	6.79090645	-0.21374254	-0.02195339
C	4.60429679	1.68457757	5.24486069
C	3.39042286	0.90725975	5.28473263
C	8.17395759	-0.36226649	0.30025262
C	7.59167503	-0.34370606	2.69563444
C	8.55588029	-0.42396672	1.59810597
C	5.72541411	0.83643120	5.58865365
C	7.10996059	1.33537637	5.84400783
C	3.76858626	-0.44556580	5.51401305
C	2.86072278	-1.62732749	5.60017449
C	5.22389176	-0.48872650	5.71384575
C	6.02327509	-1.70426431	6.03884614
Ir	4.76723804	0.20112435	3.71105288
N	3.72654839	-0.01535782	-0.27999327
N	3.69934773	0.03673989	1.93032411
N	6.25857625	-0.11973424	2.33755994
O	7.92063517	-0.46557873	3.86952730
H	1.26759143	-0.01822843	-1.75669149
H	1.12827796	-0.01004978	3.24855912
H	4.08713778	-0.05874613	-1.22176581
H	3.88654126	3.48492583	4.32890860
H	1.87635904	2.02278931	4.22216527
H	5.64511057	3.43060915	4.57483283
H	1.24778276	0.72325881	5.25559999

H	4.56394446	3.68381480	5.95382188
H	6.46015055	-0.19583937	-1.05381617
H	1.86252004	2.20440562	5.98202934
H	7.50352549	1.87982004	4.98344261
H	8.90613976	-0.43550258	-0.49692777
H	1.91419260	-1.43920350	5.09063619
H	9.59049388	-0.55307870	1.89268739
H	7.08117128	2.01111252	6.70533585
H	7.79307804	0.51434309	6.04757332
H	2.64882705	-1.85917048	6.64889195
H	3.32152793	-2.50642106	5.14536911
H	6.98852408	-1.65832782	5.53156503
H	5.50162429	-2.61296695	5.73343300
H	6.18412107	-1.75335579	7.12096974
H	-0.94600092	-0.01928721	1.93887716
C	-1.29550964	-0.01880587	-0.81805014
C	-1.33044884	1.21321081	-1.73869430
H	-0.49062293	1.22240788	-2.43957989
H	-2.25286028	1.21110513	-2.32672749
H	-1.29756689	2.13878868	-1.15632544
C	-2.54182811	0.00778450	0.07239922
H	-3.43527385	0.00482654	-0.55723347
H	-2.59486718	-0.87050150	0.72318647
H	-2.57763910	0.90880161	0.69282334
C	-1.33383122	-1.29871709	-1.67058073
H	-0.49565175	-1.34580716	-2.37191423
H	-1.29905125	-2.19072136	-1.03833823
H	-2.25796796	-1.32870648	-2.25535543

TS$_1$



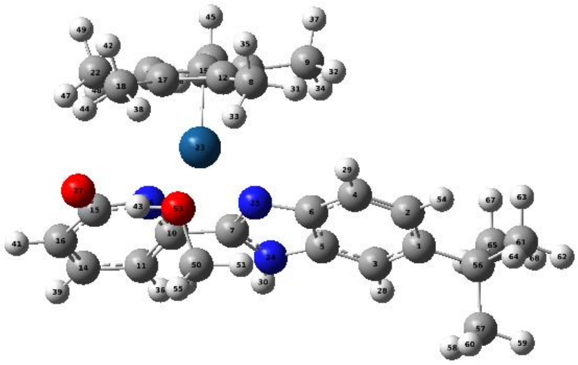
TS$_1$	
SCF Done: E (RM062X)	**-1468.112389**
Thermal correction to Gibbs Free Energy	**0.471448**

C	4.81733600	0.02196800	-0.21780300
C	4.01687300	-1.09922100	-0.54461200

C	4.19702700	1.23697700	0.06726200
C	2.63283900	-1.05255400	-0.57814200
C	2.80711800	1.28557700	0.03493200
C	2.02056100	0.16022800	-0.26448600
C	0.65903400	1.81595000	0.09610200
C	-2.74479400	-3.10106700	-1.24505100
C	0.11341900	-3.51617600	0.13388700
C	-0.62237800	2.50902500	0.16552800
C	-0.76898200	3.83447700	0.49641900
C	-2.22590300	-2.36700400	-0.05234300
C	-0.90551000	-2.48798000	0.51571100
C	-2.06975700	4.37247600	0.47081800
C	-2.89704000	2.23112600	-0.31717700
C	-3.11687400	3.58776400	0.06747400
C	-2.96126500	-1.40507800	0.70725700
C	-4.41213000	-1.08755000	0.53880200
C	-0.85711700	-1.63089500	1.69171100
C	0.33083000	-1.48294400	2.58729400
C	-2.10731700	-0.95886900	1.80369200
C	-2.51901800	0.03464500	2.84110200
Ir	-1.18357500	-0.44631900	-0.14602100
N	1.90663100	2.31800200	0.25404800
N	0.68873100	0.53097300	-0.20409100
N	-1.66116100	1.69495500	-0.18071200
O	-3.88060000	1.54164000	-0.77657800
H	4.77807900	2.12130600	0.30754800
H	2.04036600	-1.91492500	-0.86000800
H	2.13917200	3.27909900	0.45419600
H	-1.92681500	-3.50094300	-1.84715300
H	0.23112900	-3.58446900	-0.94997200
H	-3.35232200	-2.43757700	-1.86582700
H	1.08612900	-3.29328200	0.57585400
H	-3.36920800	-3.93839300	-0.91787800
H	0.08380400	4.44399000	0.77061000
H	-0.20038300	-4.49839200	0.50153000
H	-4.71487000	-1.18694200	-0.50489600
H	-2.23572100	5.40869300	0.74542700
H	1.26009300	-1.49772600	2.01145100
H	-4.13027000	3.96199800	-0.00841500
H	-5.00128700	-1.79005800	1.13771300
H	-3.67006500	0.71561900	-1.56147300
H	-4.64487700	-0.07168100	0.85716800
H	0.36273600	-2.30920500	3.30433600
H	0.29386900	-0.54779700	3.14864800
H	-3.11394300	0.83610800	2.39555300
H	-1.65537200	0.48174000	3.33606500
H	-3.13403300	-0.45470400	3.60323200
C	-2.20980400	0.01618500	-2.81060000
H	-1.20831700	-0.42709800	-1.81592700
H	-1.77673500	1.02344300	-2.86144100
O	-3.41363300	-0.13615500	-2.42290800
H	4.50103900	-2.03672000	-0.78776000
H	-1.81597200	-0.70020400	-3.53979500
C	6.34747600	-0.05619700	-0.17083700

C	6.93918500	0.94902900	-1.17377500
H	6.64883500	1.97739900	-0.93990800
H	8.03171800	0.89931800	-1.14806600
H	6.60964400	0.72517000	-2.19254200
C	6.86783400	-1.45341500	-0.52338700
H	7.95969700	-1.45464900	-0.47187500
H	6.50392000	-2.21112800	0.17758000
H	6.58532000	-1.74863100	-1.53870400
C	6.82351200	0.29422100	1.24950300
H	6.52797600	1.30691200	1.53926000
H	6.41057500	-0.40405400	1.98349800
H	7.91488900	0.23875600	1.30111500

I_1

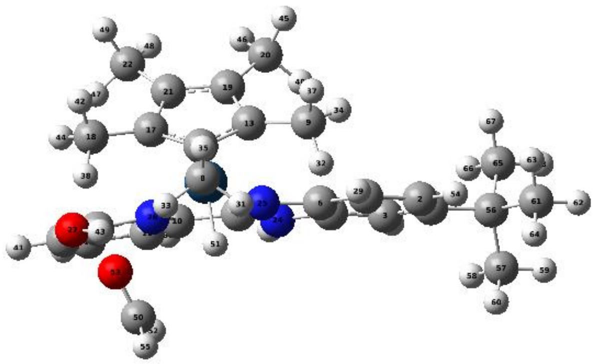


I_1	
SCF Done: E (RM062X)	**-1468.151359**
Thermal correction to Gibbs Free Energy	**0.478003**

C	4.75182100	-0.00213700	-0.09661500
C	3.95398300	-1.07973100	-0.54873000
C	4.12917200	1.17102500	0.32858300
C	2.56964700	-1.03020600	-0.57847200
C	2.73968100	1.22239300	0.29844000
C	1.95593600	0.13881700	-0.13175500
C	0.59096500	1.75896800	0.37806900
C	-1.32355100	-3.47504800	-1.34516900
C	0.44985500	-2.89878400	1.31913400
C	-0.69464800	2.45296000	0.41969900
C	-0.89214900	3.78640300	0.66590100
C	-1.66599000	-2.58727400	-0.19216700
C	-0.87693900	-2.31311600	0.95943800
C	-2.20224600	4.28967800	0.45823900
C	-2.91135900	2.10876700	-0.39108700
C	-3.18245300	3.48813600	-0.05531000
C	-2.92098000	-1.84563100	-0.06632700
C	-4.04325900	-1.86696600	-1.05244700
C	-1.58911900	-1.34764900	1.78316500
C	-1.14632900	-0.84101600	3.11845100

C	-2.88837700	-1.12813100	1.16660600
C	-3.97221100	-0.25503800	1.70705700
Ir	-1.27767000	-0.43729700	-0.09721900
N	1.83596800	2.22936500	0.61497000
N	0.62373600	0.50791400	-0.06022500
N	-1.69198500	1.62053900	0.01498000
O	-3.69179500	1.36530900	-1.02702700
H	4.70905300	2.02446000	0.66470400
H	1.97597300	-1.85879900	-0.95095000
H	2.06353300	3.15935800	0.93390300
H	-0.26474800	-3.73850100	-1.34484100
H	0.89793200	-3.43739100	0.48376600
H	-1.54908500	-2.97770100	-2.29128600
H	1.15302500	-2.13146100	1.65153600
H	-1.90651200	-4.39970900	-1.29636900
H	-0.08283500	4.43600200	0.97671200
H	0.31044400	-3.60876400	2.14073600
H	-3.66697200	-2.05671900	-2.06010000
H	-2.41304500	5.33197500	0.67469200
H	-0.05784400	-0.76453000	3.16436300
H	-4.17528000	3.86186500	-0.27584600
H	-4.74963500	-2.66316200	-0.79795200
H	-2.50436100	0.50016800	-2.11532700
H	-4.56586500	-0.90880700	-1.05844900
H	-1.47575600	-1.51757600	3.91320100
H	-1.56529300	0.14760900	3.31635100
H	-4.57207700	0.16159800	0.89737100
H	-3.55697400	0.57111600	2.28855900
H	-4.61588900	-0.84639400	2.36570700
C	-0.75741300	0.92826700	-2.97908900
H	0.20471400	0.42167200	-3.06490900
H	-0.62543800	1.87260700	-2.43987700
O	-1.63590700	0.05221300	-2.27184100
H	4.43900300	-1.98348200	-0.89578500
H	-1.15834900	1.12386100	-3.97573200
C	6.28283300	-0.07759200	-0.07291100
C	6.85633700	1.02265500	-0.98230600
H	6.56370200	2.02156600	-0.64611600
H	7.94938100	0.97737700	-0.97766900
H	6.51226800	0.89617700	-2.01296700
C	6.80545200	-1.43143800	-0.56425000
H	7.89759800	-1.43196600	-0.52017000
H	6.44950200	-2.25617600	0.06118100
H	6.51758400	-1.62704700	-1.60188700
C	6.77587800	0.13781100	1.36826800
H	6.48120000	1.11692500	1.75648600
H	6.37400700	-0.62843500	2.03775500
H	7.86802400	0.08254200	1.40147600

I_2

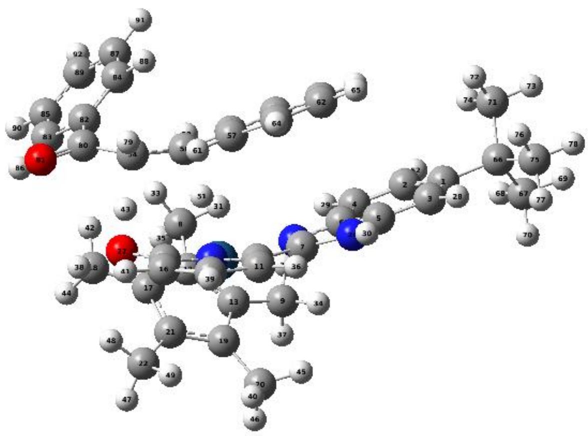


I2	
SCF Done: E (RM062X)	**-1468.124323**
Thermal correction to Gibbs Free Energy	**0.475170**

C	-4.85770800	-0.01197500	0.27293600
C	-4.02987500	-1.11989100	0.57932600
C	-4.26587800	1.20906100	-0.04201500
C	-2.64728700	-1.05459300	0.56297800
C	-2.87598700	1.27734900	-0.05639600
C	-2.06228400	0.16417800	0.21927800
C	-0.74118700	1.83855800	-0.16998900
C	2.63071500	-3.08997200	1.28090400
C	-0.17628600	-3.45211600	-0.15578800
C	0.52371700	2.55684200	-0.23478600
C	0.65752000	3.89888000	-0.52268400
C	2.16068100	-2.32649700	0.08454500
C	0.86415900	-2.44052200	-0.52707000
C	1.94276200	4.45511400	-0.47723500
C	2.78494700	2.31020300	0.19531200
C	3.00936400	3.66843700	-0.10701700
C	2.93219500	-1.41342300	-0.70126000
C	4.40029700	-1.15157800	-0.55276300
C	0.89902800	-1.69478100	-1.78857400
C	-0.26316100	-1.60191600	-2.72667800
C	2.14727400	-1.06621100	-1.88996000
C	2.64412500	-0.16268100	-2.97459600
Ir	1.15482000	-0.39345100	0.11145200
N	-2.00079500	2.32446300	-0.29644400
N	-0.73884900	0.55275900	0.12132400
N	1.57704000	1.75352000	0.07681900
O	3.81225800	1.58986100	0.60281800
H	-4.86693300	2.08459200	-0.26518900
H	-2.03261200	-1.90383800	0.83319700
H	-2.25560000	3.28077700	-0.49065100
H	1.81353000	-3.25811500	1.98510900
H	-0.31815000	-3.50589300	0.92621600
H	3.42915100	-2.55809600	1.79929500
H	-1.13645200	-3.22577600	-0.62367100

H	3.01343300	-4.06523900	0.96211700
H	-0.20399300	4.50445800	-0.77762300
H	0.13422700	-4.44315300	-0.50375100
H	4.71336400	-1.19247700	0.49175000
H	2.09291600	5.50350400	-0.71023600
H	-1.18830600	-1.39053300	-2.18064300
H	4.01783200	4.05206400	-0.01805500
H	4.95495100	-1.91982700	-1.10189400
H	3.54112400	0.73881000	1.01419100
H	4.68303500	-0.17849000	-0.95793700
H	-0.39952400	-2.54976900	-3.25699800
H	-0.11929300	-0.81641600	-3.47010000
H	3.12870800	0.72423400	-2.55572400
H	1.83550400	0.16664600	-3.62884000
H	3.38736500	-0.68166500	-3.58846300
C	3.24430100	0.00867700	3.54085100
H	1.10419100	-0.31297600	1.67526900
H	2.48711400	0.81067500	3.49450300
O	3.85513700	-0.33986100	2.55778600
H	-4.49169900	-2.06147100	0.84885100
H	3.41656800	-0.46506800	4.52013900
C	-6.38736200	-0.11069300	0.28861700
C	-6.94918400	0.88529800	1.31778800
H	-6.68132700	1.91744100	1.07384400
H	-8.04117400	0.82180600	1.33875200
H	-6.57335200	0.66430100	2.32109400
C	-6.87506100	-1.51483600	0.65949900
H	-7.96796300	-1.53107800	0.64756300
H	-6.52570100	-2.26753800	-0.05411500
H	-6.55174800	-1.80574700	1.66376000
C	-6.92767400	0.23588800	-1.10939900
H	-6.65614200	1.25209600	-1.40966000
H	-6.53837900	-0.45679400	-1.86134600
H	-8.01964200	0.16824600	-1.11425500

TS$_2$



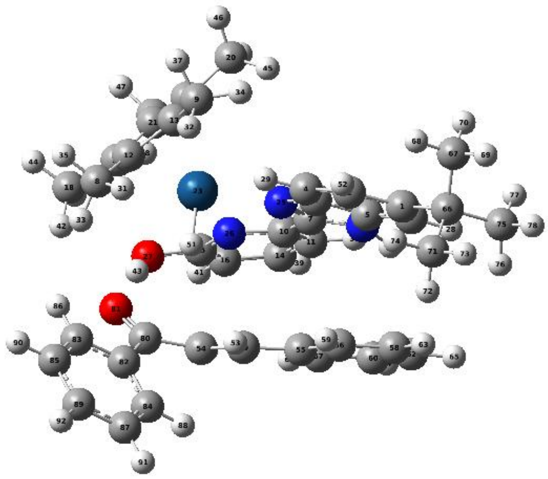
TS$_2$

SCF Done: E (RM062X)	**-2007.106661**
Thermal correction to Gibbs Free Energy	**0.691667**

C	5.08820300	0.98642800	-0.41278700
C	4.03333500	1.56271600	-1.17163500
C	4.82771400	-0.13483000	0.36441100
C	2.75232100	1.04956300	-1.19444600
C	3.53006400	-0.64945500	0.34793300
C	2.50337300	-0.09334500	-0.42802600
C	1.62954200	-1.70962900	0.72969700
C	-1.81182300	1.77641900	-2.51009600
C	0.66281900	0.10165200	-3.75861600
C	0.54985100	-2.49507700	1.31963000
C	0.68962000	-3.47008500	2.28336900
C	-1.61401500	0.29345000	-2.47324000
C	-0.50163000	-0.44045000	-2.99273000
C	-0.48582300	-4.00729500	2.83479100
C	-1.79071000	-2.46925700	1.49821800
C	-1.71323900	-3.50880300	2.46106700
C	-2.56060800	-0.65961100	-1.91277000
C	-3.91725600	-0.33447600	-1.37894000
C	-0.73227400	-1.85268200	-2.75375600
C	0.15699800	-2.97083400	-3.19219500
C	-2.01170000	-1.97106000	-2.10229300
C	-2.66087100	-3.25079300	-1.68498500
Ir	-0.66604700	-0.78179600	-0.83086100
N	2.94026200	-1.68111900	1.05934900
N	1.33785300	-0.79077800	-0.17552200
N	-0.65844900	-2.06102900	0.88475800
O	-2.90741400	-1.87850100	1.21185500
H	5.59439000	-0.59437800	0.97657600
H	1.95459700	1.52399200	-1.75551200
H	3.37813100	-2.23171500	1.78251900
H	-0.85582300	2.30271000	-2.55234600
H	0.72079400	1.18876300	-3.68683000
H	-2.35449000	2.12471100	-1.62594000
H	1.60860000	-0.32212000	-3.41214400
H	-2.39626300	2.05534400	-3.39265500
H	1.66718000	-3.80437800	2.60992400
H	0.54470000	-0.15533900	-4.81624300
H	-4.17634300	-0.95709400	-0.52136500
H	-0.42139600	-4.78916800	3.58429200
H	0.03512900	-3.84439000	-2.54856500
H	-2.64021200	-3.85258600	2.90343200
H	-3.96689900	0.71062900	-1.07078900
H	-2.79991500	-0.72229700	1.43963700
H	-4.66663300	-0.48519300	-2.16319100
H	1.20695200	-2.67040400	-3.16524500
H	-0.08244100	-3.27094600	-4.21794300
H	-3.16245600	-3.69995300	-2.54823100

H	-3.39881200	-3.07291800	-0.90203700
H	-1.92368600	-3.96743400	-1.31410100
C	-1.30232400	1.07333200	1.46573100
H	-0.97071100	0.38072000	0.36749200
H	4.24305900	2.45311200	-1.75508600
H	-1.31673400	1.99187000	0.87767300
C	-2.57168300	0.60764200	1.96517800
C	-0.04169300	0.91772400	2.24880900
C	1.06514600	1.70155700	1.90318700
C	0.08940800	-0.01353800	3.28484800
C	2.27532400	1.56478400	2.57311200
H	0.97608300	2.41647400	1.08785600
C	1.29939400	-0.15029000	3.96017500
H	-0.75116200	-0.64184400	3.56620300
C	2.39459700	0.63575500	3.60616500
H	3.12482500	2.17649000	2.28466900
H	1.38212900	-0.86826500	4.77019400
H	3.33463200	0.53380700	4.13954200
C	6.47299000	1.63487700	-0.46994300
C	6.97176800	1.62879400	-1.92560900
H	6.31268800	2.20049700	-2.58481900
H	7.96703100	2.07987700	-1.97935000
H	7.03747300	0.60733900	-2.31157000
C	6.37483700	3.08463000	0.03502000
H	6.02361400	3.11405200	1.07112600
H	7.35981300	3.55934500	-0.00537100
H	5.69263600	3.68420300	-0.57388600
C	7.49328700	0.88848200	0.39435000
H	7.20924300	0.89179500	1.45173900
H	7.62016500	-0.14831900	0.06658900
H	8.46591300	1.38055800	0.31398400
H	-2.57741300	0.21121500	2.98054700
C	-3.86202900	1.25696500	1.61979700
O	-4.91545400	0.69072600	1.85923800
C	-3.90760200	2.60567700	0.94210700
C	-4.93994900	2.83766900	0.02702900
C	-3.03518400	3.65028700	1.26337200
C	-5.05690400	4.06863000	-0.60827300
H	-5.65496400	2.04093100	-0.15652700
C	-3.16575600	4.89116300	0.64453500
H	-2.27966100	3.50923100	2.03196200
C	-4.16420000	5.09548400	-0.30491300
H	-5.85414400	4.23547100	-1.32515800
H	-2.49734900	5.70256600	0.91329500
H	-4.26126700	6.06105100	-0.79059400

I_3



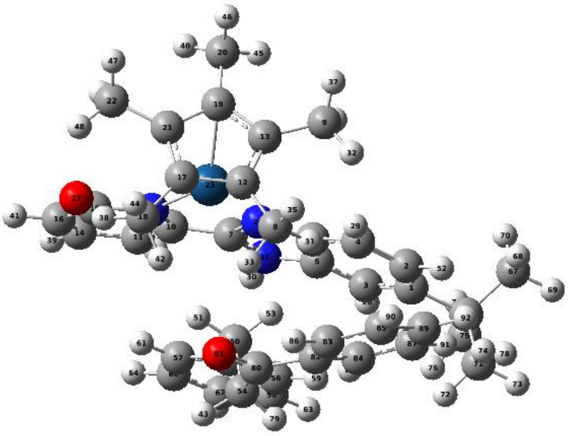
I$_3$	
SCF Done: E (RM062X)	**-2007.180853**
Thermal correction to Gibbs Free Energy	**0.691260**

C	4.75555900	-0.34960700	-1.15597200
C	3.72343800	-0.33650000	-2.13418300
C	4.42373000	-0.56834700	0.17412500
C	2.39319500	-0.54382200	-1.83110900
C	3.07750600	-0.77323700	0.48361900
C	2.06795400	-0.77824800	-0.49050500
C	1.10579300	-1.03204800	1.43085200
C	-2.64321800	-0.20592300	-3.20036800
C	-0.25027300	-2.35365400	-3.31315300
C	0.00138800	-1.07279400	2.37713700
C	0.13772300	-1.33354200	3.72643600
C	-2.37250600	-1.29126400	-2.20782500
C	-1.27797700	-2.22146600	-2.23334800
C	-1.01217300	-1.27871100	4.52156200
C	-2.26651600	-0.65244000	2.56389700
C	-2.21321600	-0.92362400	3.94608200
C	-3.19163500	-1.61454300	-1.07343200
C	-4.52618200	-1.00675200	-0.76676100
C	-1.50959600	-3.22657100	-1.19416800
C	-0.61588700	-4.40259300	-0.95344300
C	-2.66142800	-2.84918600	-0.48903400
C	-3.25839500	-3.52393700	0.70512100
Ir	-1.19077300	-1.04629000	-0.41670500
N	2.43270000	-0.95382900	1.69419800
N	0.85243100	-0.96262000	0.13960800
N	-1.18590100	-0.78467600	1.78267100
O	-3.41663500	-0.27023300	2.04555700
H	5.17147500	-0.57114700	0.95849800
H	1.61818600	-0.50222400	-2.58726600
H	2.83388600	-0.76944700	2.60412100

H	-1.71932100	0.16347600	-3.64880300
H	-0.09366600	-1.40541700	-3.83143900
H	-3.14257400	0.63677800	-2.72030000
H	0.70845500	-2.69597200	-2.91599200
H	-3.29017000	-0.58372300	-3.99876000
H	1.10594200	-1.58168300	4.14564400
H	-0.58734700	-3.08729500	-4.05335100
H	-4.82891300	-1.21186400	0.26102400
H	-0.95607700	-1.49300700	5.58337200
H	-0.82207600	-4.87294800	0.00952300
H	-3.12890300	-0.82388500	4.51554400
H	-4.50652900	0.07727400	-0.89816300
H	-3.30084900	0.40752100	1.31081800
H	-5.28672700	-1.42393000	-1.43527300
H	0.43676800	-4.10558700	-0.96879100
H	-0.75823300	-5.15812700	-1.73302800
H	-4.09897400	-4.15577900	0.40045100
H	-3.64209100	-2.78434000	1.41236900
H	-2.52880200	-4.15261400	1.21909100
C	0.02629700	2.55066600	1.05354100
H	-1.01330900	0.48192400	-0.66738900
H	3.99143100	-0.14520800	-3.16828000
H	0.27091800	2.83396200	0.03037200
C	-1.26898100	2.44524800	1.38731400
C	1.18279100	2.26677400	1.91471300
C	2.46753400	2.36518300	1.36407800
C	1.05677100	1.90408400	3.26493100
C	3.59878200	2.12526400	2.13937400
H	2.57887500	2.63325900	0.31641600
C	2.18368200	1.65232300	4.03650500
H	0.07292100	1.81893600	3.71797700
C	3.46097800	1.76755300	3.47821200
H	4.58463600	2.21761200	1.69433300
H	2.07031000	1.38667800	5.08310500
H	4.33999100	1.59507800	4.09161800
C	6.19757500	-0.10221700	-1.60360500
C	6.60371100	-1.18031000	-2.62278300
H	5.96551900	-1.16255700	-3.51027500
H	7.63453000	-1.01410700	-2.95010300
H	6.54096900	-2.17825200	-2.17906200
C	6.29088200	1.28735200	-2.25708800
H	5.99620300	2.07012800	-1.55075100
H	7.31954200	1.48268700	-2.57499200
H	5.64909100	1.36624200	-3.13865100
C	7.18035400	-0.15203600	-0.43048100
H	6.96205800	0.62052600	0.31466400
H	7.17106800	-1.12870200	0.06384900
H	8.19467600	0.02320300	-0.79819700
H	-1.58551100	2.10150200	2.36950700
C	-2.36031200	2.56660700	0.39350900
O	-3.29548400	1.76344900	0.43261600
C	-2.33977200	3.61409500	-0.65725500
C	-3.19603200	3.44899100	-1.75340900
C	-1.55115700	4.76705100	-0.56206300

C	-3.23625500	4.40175100	-2.75993000
H	-3.83273300	2.57148300	-1.78541800
C	-1.60152000	5.72597300	-1.56877500
H	-0.92509400	4.92871500	0.30867900
C	-2.43443000	5.54020700	-2.66896400
H	-3.89723200	4.26796100	-3.60952500
H	-0.99856000	6.62408600	-1.48972100
H	-2.47097800	6.29075500	-3.45202100

I$_4$



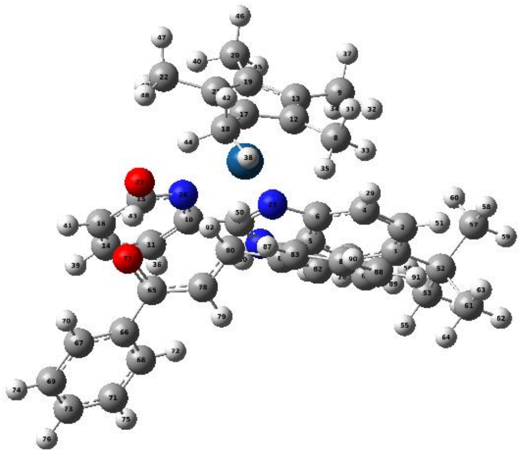
I$_4$	
SCF Done: E (RM062X)	**-2007.185509**
Thermal correction to Gibbs Free Energy	**0.695661**

C	3.95051400	-1.07226900	-1.55703900
C	3.30758700	0.19004500	-1.63745800
C	3.18823400	-2.20010500	-1.27582000
C	1.94657300	0.35762400	-1.45856300
C	1.81905500	-2.02769200	-1.07896000
C	1.18800400	-0.78167400	-1.18169500
C	-0.31185400	-2.22965800	-0.53876600
C	-0.60887300	3.15273500	0.01314600
C	-0.62280700	2.18323600	-3.05783200
C	-1.59676800	-2.65981500	-0.01121600
C	-1.89755700	-3.93863000	0.34415700
C	-1.67393800	2.35962100	-0.66454900
C	-1.67144100	1.93472200	-2.01880400
C	-3.15892300	-4.17168300	0.97023200
C	-3.64870200	-1.75770000	0.84657800
C	-3.99121100	-3.13059100	1.21850400
C	-2.95309300	1.96307900	-0.05943800
C	-3.35750400	2.21829200	1.35324000
C	-2.91240700	1.23080500	-2.24969100
C	-3.32677100	0.61507100	-3.54254400
C	-3.73505900	1.32184600	-1.06113400

C	-5.15875700	0.87529200	-0.98831700
Ir	-1.88607600	0.18935200	-0.70571000
N	0.83092800	-2.92190000	-0.69007200
N	-0.15197200	-0.94853600	-0.85967500
N	-2.44079600	-1.58797100	0.16373300
O	-4.36485900	-0.79948300	1.11280700
H	3.63413600	-3.18258100	-1.17910100
H	1.48619000	1.33735000	-1.51030200
H	0.99334100	-3.85266000	-0.32837200
H	0.39402600	2.78909100	-0.22681300
H	0.21104200	2.75280800	-2.64409700
H	-0.72814500	3.13554700	1.09686500
H	-0.23431000	1.25218200	-3.47936700
H	-0.67224300	4.19726500	-0.31194300
H	-1.19391000	-4.74615900	0.17935100
H	-1.05219600	2.77105000	-3.87484500
H	-4.00657600	1.41291300	1.70049100
H	-3.43791600	-5.18078700	1.25556400
H	-4.02888000	-0.20462500	-3.38051000
H	-4.94953100	-3.25889500	1.70775200
H	-2.48647200	2.27838700	2.01157700
H	0.68092300	0.65803200	4.28396900
H	-3.89268300	3.17192100	1.41503200
H	-2.46351300	0.23880900	-4.09533600
H	-3.82414200	1.37201900	-4.15943000
H	-5.74679700	1.47867500	-1.68797400
H	-5.55840600	0.99194400	0.01610900
H	-5.26277100	-0.17733400	-1.25863200
C	0.59101100	0.05895300	2.19744800
H	-0.50235300	0.15356100	2.21398600
H	3.90764500	1.06992500	-1.84704500
H	0.93301500	0.46938900	1.23673300
C	1.17476300	0.91218300	3.34370100
C	0.99684600	-1.38986000	2.28851400
C	2.30508000	-1.76992200	1.96771900
C	0.09662200	-2.37317900	2.70375300
C	2.70358800	-3.09985400	2.05171600
H	3.01293800	-1.01671200	1.62299300
C	0.48742200	-3.70877200	2.78076200
H	-0.92448400	-2.09326900	2.95475500
C	1.79151200	-4.07713800	2.45350300
H	3.72462400	-3.37410600	1.80229900
H	-0.22598400	-4.45917100	3.10784000
H	2.10247300	-5.11418100	2.53282100
C	5.46635300	-1.14369000	-1.75285900
C	5.82762700	-0.60382600	-3.14705600
H	5.52358800	0.43903900	-3.27221900
H	6.91028400	-0.65469400	-3.29657700
H	5.34533200	-1.19470700	-3.93110700
C	6.15034700	-0.28646100	-0.67386100
H	5.89084700	-0.64043500	0.32924700
H	7.23740800	-0.34110000	-0.78457800
H	5.86212900	0.76609800	-0.74984100
C	5.99353200	-2.57696900	-1.63707700

H	5.80233100	-3.00038900	-0.64532800
H	5.54943300	-3.23391900	-2.39157300
H	7.07537900	-2.57945900	-1.79227500
H	2.24647500	0.72438700	3.44974400
C	0.88180900	2.36210700	3.02833800
O	-0.18603000	2.85312500	3.34863800
C	1.85357200	3.14485100	2.19850500
C	1.63060300	4.51878500	2.05335700
C	2.90891100	2.54153500	1.50632500
C	2.45017000	5.27928700	1.22957500
H	0.80478000	4.96759600	2.59655100
C	3.71957000	3.30285700	0.66799400
H	3.09905000	1.47622300	1.60045400
C	3.49285000	4.66996500	0.53065900
H	2.28185000	6.34662200	1.13145000
H	4.53785200	2.82922700	0.13478800
H	4.13314200	5.26433000	-0.11313600

TS_3



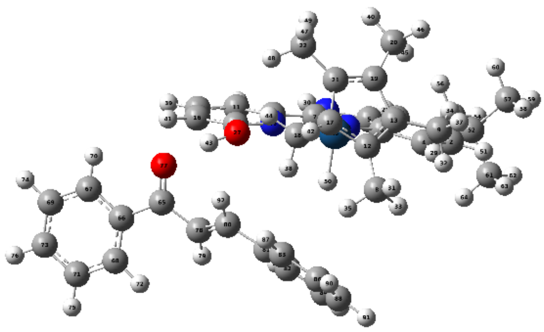
TS_3	
SCF Done: E (RM062X)	**-2007.143382**
Thermal correction to Gibbs Free Energy	**0.691075**

C	-4.78155700	2.02417800	-0.31278300
C	-4.48404900	0.87291300	0.46719100
C	-3.82615900	2.51050300	-1.19597700
C	-3.28942100	0.18912600	0.37517100
C	-2.61249100	1.82438200	-1.28434100
C	-2.34418700	0.66784500	-0.53828500
C	-0.56492700	1.09865700	-1.70712500
C	-1.24931800	-3.15272000	2.01528900
C	-2.85309100	-2.94434200	-0.78734200
C	0.84175600	0.97890900	-2.06738300
C	1.58094500	1.94479800	-2.71751500

C	-0.66123500	-3.16490000	0.63992900
C	-1.37478700	-3.09328900	-0.60380100
C	2.97199000	1.77524100	-2.77226000
C	2.73565900	-0.25073000	-1.46847300
C	3.54762600	0.69706700	-2.14062500
C	0.74221000	-3.39356900	0.31854700
C	1.84488000	-3.59056500	1.30763500
C	-0.44512000	-3.24174200	-1.68738300
C	-0.78667200	-3.30887300	-3.14108000
C	0.86710200	-3.43163900	-1.10555900
C	2.10788000	-3.70854700	-1.89201500
Ir	0.12690500	-1.46292500	-0.47014100
N	-1.45951100	2.06931600	-2.01469900
N	-1.06698400	0.23527900	-0.84085700
N	1.39380000	-0.13543900	-1.51900700
O	3.24602200	-1.19599100	-0.73198600
H	-4.00426000	3.39590500	-1.79399200
H	-3.06228800	-0.66839200	0.99979900
H	-1.30862900	2.83489200	-2.65391100
H	-1.42167600	-4.17687500	2.36242600
H	-3.36611900	-2.80784300	0.16475500
H	-2.20407800	-2.62369400	2.03508800
H	-3.09908500	-2.09918100	-1.43573700
H	-0.58703900	-2.65420400	2.72669800
H	1.10759400	2.82716100	-3.13203100
H	-3.24797700	-3.85316700	-1.25211900
H	1.59410400	-3.12054800	2.26280600
H	3.59215100	2.51442800	-3.26767400
H	0.04320500	-2.95649600	-3.75692600
H	4.62152000	0.56198100	-2.09326300
H	2.00592100	-4.65763100	1.49048000
H	3.83357000	-0.64545400	0.07601500
H	2.77527200	-3.15463800	0.93542100
H	-1.66538100	-2.70146800	-3.36898000
H	-1.00611700	-4.34158800	-3.43418800
H	2.07295600	-4.73866600	-2.26147000
H	3.00233200	-3.57445200	-1.28681800
H	2.18384800	-3.04226300	-2.75537000
H	0.87532300	-0.61437700	0.78000700
H	-5.22894600	0.51737300	1.17161000
C	-6.14488700	2.69743500	-0.13958300
C	-6.30625300	3.91224700	-1.05827200
H	-7.29352700	4.35533400	-0.90443700
H	-5.56163700	4.68564700	-0.84378600
H	-6.23069600	3.63307400	-2.11419300
C	-7.25356200	1.68511800	-0.47521100
H	-7.22520500	0.81381500	0.18492300
H	-8.23369500	2.15728300	-0.36024200
H	-7.16154900	1.33319100	-1.50702500
C	-6.29723600	3.16606500	1.31780000
H	-7.26970100	3.64891400	1.45227200
H	-6.23990100	2.33245500	2.02329900
H	-5.51742100	3.88773900	1.57881400
C	3.55255300	1.24670400	1.00282600

C	4.15737600	2.57642500	0.72456800
C	5.55257200	2.68412900	0.71728000
C	3.38023800	3.70006500	0.41840700
C	6.15947300	3.90207000	0.43741500
H	6.14095400	1.80118200	0.94122800
C	3.99039600	4.91387500	0.12443500
H	2.29808200	3.62235000	0.38077500
C	5.37982900	5.01890800	0.14124800
H	7.24125500	3.98278700	0.44979700
H	3.38371200	5.78024500	-0.11769000
H	5.85449100	5.96971400	-0.07837700
O	4.31467000	0.22821500	0.84426600
C	2.21977800	1.15390400	1.45951900
H	1.65431300	2.05984600	1.64176900
C	1.67490000	-0.08119600	1.84572300
C	0.61804700	-0.16817000	2.89511400
C	-0.62916500	0.44205400	2.73540200
C	0.88587800	-0.88328400	4.06455100
C	-1.59597300	0.33330200	3.72772800
H	-0.84373300	0.97991300	1.81464200
C	-0.08183100	-0.98584500	5.06337700
H	1.85862700	-1.34975400	4.19801100
C	-1.32470800	-0.38351100	4.89427000
H	-2.56426100	0.80497800	3.58911300
H	0.13771200	-1.53896300	5.97049300
H	-2.08024100	-0.47064600	5.66788100
H	2.39112600	-0.90458200	1.85423300

I$_5$



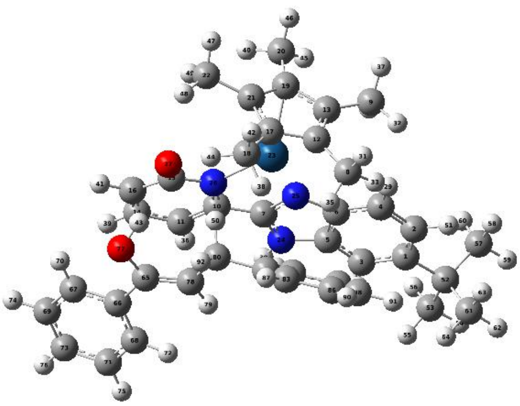
I$_5$	
SCF Done: E (RM062X)	**-2007.253181**
Thermal correction to Gibbs Free Energy	**0.676293**

C	-5.83303000	1.71006500	1.10291700
C	-5.41678400	0.35927600	1.24910900
C	-4.95368500	2.63017900	0.54987000
C	-4.17877300	-0.09820700	0.84717400

C	-3.69892600	2.16801600	0.14659000
C	-3.30699600	0.82480500	0.25916400
C	-1.63565600	1.90332900	-0.59270200
C	-0.06426500	-3.74380200	0.80593300
C	-3.04859400	-3.19206200	-0.21773000
C	-0.27344600	2.12128600	-1.05026700
C	0.25298100	3.36639200	-1.33723300
C	-0.45967300	-3.03255900	-0.44885500
C	-1.79121500	-2.70733400	-0.86966100
C	1.60114700	3.43825100	-1.69326200
C	1.73775800	1.04823900	-1.43554900
C	2.34987100	2.28283700	-1.74158600
C	0.44147100	-2.58803400	-1.46904700
C	1.89548800	-2.93864100	-1.52041800
C	-1.71661600	-2.16644900	-2.22833600
C	-2.91361800	-1.74370200	-3.02176200
C	-0.36210100	-2.09015100	-2.58608700
C	0.22538800	-1.55653400	-3.85454800
Ir	-0.63395300	-0.87683400	-0.61958700
N	-2.61046900	2.82639900	-0.39426900
N	-2.02077900	0.69565400	-0.23313300
N	0.44393800	0.97127500	-1.10040900
O	2.39760000	-0.09143200	-1.48252200
H	-5.21735200	3.67482800	0.43712100
H	-3.87223300	-1.12342800	1.00269500
H	-2.55124200	3.81196200	-0.59773800
H	0.01162000	-4.82055000	0.61842000
H	-2.97597300	-3.16196100	0.87185400
H	-0.79571900	-3.58249700	1.60011400
H	-3.91555000	-2.60644100	-0.52997800
H	0.90380200	-3.38647400	1.16309000
H	-0.35762400	4.25925800	-1.27765600
H	-3.23041900	-4.23172300	-0.51125100
H	2.36562000	-2.77301700	-0.54913000
H	2.05623800	4.39395700	-1.92966800
H	-2.62754800	-1.16479100	-3.90137600
H	3.39837200	2.28845500	-2.01464600
H	2.00221800	-3.99884600	-1.77638000
H	3.38603300	0.07553000	-1.43181100
H	2.42581800	-2.34774100	-2.26634300
H	-3.58707000	-1.12969800	-2.41554300
H	-3.47717400	-2.61844000	-3.36269100
H	0.54267800	-2.38143700	-4.50093500
H	1.10572100	-0.94514300	-3.63894800
H	-0.49214800	-0.94924500	-4.40897300
H	-0.14643600	-0.65073600	0.85226100
H	-6.10144100	-0.34651500	1.70820400
C	-7.23277200	2.10575900	1.57686600
C	-7.51900000	3.59243300	1.34459600
H	-8.52921200	3.82599200	1.69072700
H	-6.82444100	4.22980000	1.90130800
H	-7.46449900	3.85460300	0.28304500
C	-8.27787900	1.28336100	0.80370000
H	-8.15518200	0.20978400	0.97076400

H	-9.28477600	1.55907300	1.13151700
H	-8.20358100	1.47116100	-0.27156600
C	-7.35951700	1.81688800	3.08241800
H	-8.35680000	2.10056700	3.43204900
H	-7.21657500	0.75659200	3.30786600
H	-6.62057300	2.38788500	3.65240400
C	5.03637500	0.90958200	0.11981400
C	5.95320200	2.01947100	0.46914800
C	6.43679500	2.83088900	-0.56527400
C	6.35919200	2.26107100	1.78685500
C	7.29846800	3.88084900	-0.28355100
H	6.13402300	2.61294200	-1.58404200
C	7.22680100	3.31088900	2.06530700
H	6.02227900	1.62023200	2.59462800
C	7.69115500	4.12274000	1.03309900
H	7.67086800	4.50872600	-1.08578500
H	7.54566400	3.49232500	3.08590000
H	8.36722100	4.94243200	1.25373700
O	4.85062000	0.62217300	-1.07250100
C	4.34812100	0.15477400	1.18233900
H	4.16173700	0.63349900	2.13753100
C	4.02282800	-1.13294300	0.97179300
C	3.34287800	-2.01768400	1.92076400
C	2.44079000	-1.52487200	2.87427100
C	3.60491900	-3.39428800	1.87710600
C	1.83617900	-2.38903600	3.77851800
H	2.19584000	-0.46702800	2.88484200
C	3.01133000	-4.25549300	2.79326900
H	4.29378200	-3.78253800	1.13138400
C	2.12770100	-3.75301000	3.74660400
H	1.13329100	-2.00049200	4.50780100
H	3.23538900	-5.31643700	2.76278600
H	1.65991000	-4.42457000	4.45905600
H	4.33546700	-1.58230100	0.02825900

I_6



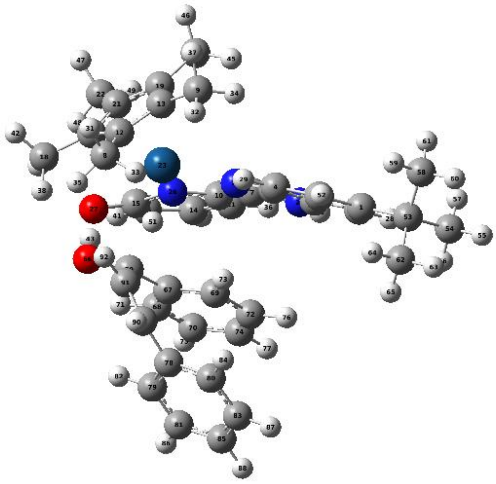
I_6

SCF Done: E (RM062X)	-2007.248062
Thermal correction to Gibbs Free Energy	0.671993

C	-4.67564100	2.30358200	-0.45578500
C	-4.65833100	0.97346900	0.03713500
C	-3.52880000	2.81639700	-1.05041700
C	-3.55446800	0.14695400	-0.05471700
C	-2.41478100	1.98192100	-1.13834300
C	-2.41188200	0.66186800	-0.66960500
C	-0.40923200	1.09006400	-1.42876100
C	-1.60928300	-2.76352600	2.14876200
C	-3.07321600	-3.20446200	-0.72661000
C	1.00912900	0.85132700	-1.63940300
C	1.86817000	1.73588700	-2.21964100
C	-0.96723700	-3.09433900	0.84368000
C	-1.61053200	-3.25616900	-0.41306800
C	3.23675200	1.35835400	-2.32961900
C	2.73386800	-0.69337200	-1.07780400
C	3.64888700	0.18008700	-1.79812700
C	0.46465000	-3.36980900	0.66281100
C	1.47939200	-3.40401600	1.75409900
C	-0.58083700	-3.53470100	-1.38977900
C	-0.81277600	-3.76983700	-2.84379600
C	0.69004100	-3.67683900	-0.70522200
C	1.95474700	-4.13695600	-1.35203800
Ir	-0.11859900	-1.64681700	-0.53745500
N	-1.13045300	2.21121000	-1.61763300
N	-1.14714500	0.12922800	-0.88074000
N	1.38504300	-0.37234200	-1.13537200
O	3.12453600	-1.66651700	-0.41842000
H	-3.48743800	3.83141600	-1.42641000
H	-3.55884000	-0.85337500	0.35854900
H	-0.77939400	3.08040300	-1.99268300
H	-1.81761200	-3.68766400	2.69864800
H	-3.66353200	-3.00758700	0.16927100
H	-2.54847900	-2.22518600	2.00834000
H	-3.30595500	-2.44214600	-1.47487000
H	-0.95807700	-2.13776300	2.76339700
H	1.52289100	2.69151800	-2.59645400
H	-3.38931500	-4.17453400	-1.12196900
H	1.19039100	-2.74823900	2.57890000
H	3.94600100	2.03005000	-2.80176200
H	0.05866600	-3.48053100	-3.43373200
H	4.68706900	-0.12980000	-1.81275900
H	1.55223900	-4.42667300	2.13980700
H	4.27753200	-0.54960700	0.90302000
H	2.45274200	-3.09255100	1.37278300
H	-1.68126600	-3.21262200	-3.20025900
H	-0.99808300	-4.83656400	-3.01217000
H	1.85777200	-5.20166700	-1.58951200
H	2.81210900	-3.98375700	-0.70092000

H	2.14648900	-3.59498500	-2.28094200
H	2.08789000	-0.82342900	1.45187200
H	-5.55163000	0.58696400	0.51691400
C	-5.95257400	3.13275000	-0.30092300
C	-5.79988600	4.53666700	-0.89359000
H	-6.73590000	5.08644600	-0.76691200
H	-5.01249000	5.10628900	-0.38952600
H	-5.57951200	4.50178000	-1.96533600
C	-7.10776700	2.42055200	-1.02576600
H	-7.30135800	1.42889800	-0.60741700
H	-8.02576700	3.00742500	-0.92687800
H	-6.88851400	2.30441100	-2.09119100
C	-6.28776300	3.26816700	1.19454700
H	-7.19747100	3.86329400	1.31795000
H	-6.46108800	2.29519900	1.66256100
H	-5.47639300	3.76653800	1.73325100
C	3.91340800	1.33828100	1.08144300
C	4.48953100	2.58639800	0.52712400
C	5.65097000	2.52233100	-0.25142600
C	3.88907500	3.83417600	0.73664800
C	6.18000200	3.67153600	-0.83133900
H	6.13460100	1.56212200	-0.39089800
C	4.41483100	4.97940800	0.15139300
H	3.02099100	3.91807200	1.38250900
C	5.55916600	4.90280000	-0.64065000
H	7.08412500	3.60597700	-1.42829000
H	3.94104400	5.93969700	0.32854200
H	5.97324900	5.79995100	-1.08894000
O	4.77017800	0.28048300	1.00553200
C	2.67806100	1.22937700	1.59826700
H	2.03111200	2.09855200	1.60255500
C	2.17123800	-0.04306700	2.22436300
C	0.82549900	0.08229900	2.89935600
C	-0.24366900	0.70934100	2.24894600
C	0.60227900	-0.45270700	4.17067300
C	-1.50000500	0.79478000	2.84399900
H	-0.07487300	1.15831400	1.27331600
C	-0.65287200	-0.36854100	4.77403600
H	1.42514800	-0.92637500	4.70022800
C	-1.70853700	0.25303600	4.11177300
H	-2.31121800	1.29903800	2.32591200
H	-0.80016300	-0.77987000	5.76755000
H	-2.68154300	0.32974500	4.58586500
H	2.90848000	-0.42148400	2.94571300

TS_4



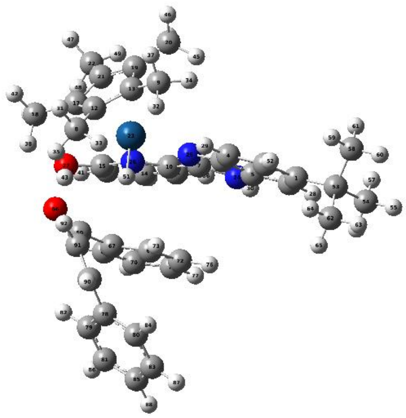
TS4	
SCF Done: E (RM062X)	-2007.139269
Thermal correction to Gibbs Free Energy	0.694404

C	4.32562900	-2.13187900	0.26608300
C	3.51847200	-2.19656500	-0.90097500
C	3.75118000	-1.72780200	1.46504200
C	2.17240900	-1.88850300	-0.90608600
C	2.39190000	-1.40919800	1.46066900
C	1.59753500	-1.50073100	0.30808400
C	0.32923000	-0.74409700	1.90239900
C	-1.84611500	-1.27506100	-3.60670700
C	-0.61995300	-3.68977500	-1.89814000
C	-0.84659000	-0.09745200	2.47082900
C	-0.97127600	0.31697200	3.77460800
C	-2.27334100	-1.69598700	-2.23639200
C	-1.71789800	-2.76653800	-1.47394500
C	-2.14212000	1.02434300	4.11727900
C	-2.83423500	0.96578300	1.78201400
C	-3.05518900	1.34158900	3.14766400
C	-3.38412400	-1.13151300	-1.48572900
C	-4.30256600	-0.04823400	-1.95203400
C	-2.47844100	-2.89688000	-0.24515000
C	-2.26662300	-3.94028800	0.80468100
C	-3.51266700	-1.89835700	-0.27605300
C	-4.54250100	-1.68619900	0.78611500
Ir	-1.54816000	-0.89683900	-0.32808200
N	1.54892500	-0.93727400	2.45497600
N	0.31592600	-1.09523100	0.62855200
N	-1.78449300	0.13803700	1.51361100
O	-3.56757200	1.39653200	0.83931800
H	4.33134800	-1.65153600	2.37677400
H	1.57791000	-1.92043300	-1.81286700
H	1.81331800	-0.68767000	3.39585900
H	-2.23241500	-1.97994300	-4.34981000

H	-0.09217600	-3.30425400	-2.77233600
H	-0.75806600	-1.24035900	-3.69802900
H	0.10650800	-3.85388600	-1.09824000
H	-2.24474100	-0.28863900	-3.84880500
H	-0.20231800	0.10938900	4.50920000
H	-1.04863100	-4.66028000	-2.16877300
H	-3.76196900	0.70228000	-2.53192300
H	-2.30160400	1.34153000	5.14271600
H	-2.59853300	-3.58751100	1.78319800
H	-3.94319100	1.92556000	3.35749900
H	-5.09696500	-0.47031500	-2.57584700
H	-2.87473600	1.93091400	-0.25796900
H	-4.75128700	0.46550700	-1.10056800
H	-1.21054900	-4.20998200	0.87944200
H	-2.83039400	-4.84759100	0.56348400
H	-5.38805600	-2.35827400	0.60776100
H	-4.90363400	-0.65721900	0.78012800
H	-4.13837100	-1.90619800	1.77716000
C	-1.07528100	2.03115800	-1.09406300
H	-0.95359200	0.53142100	-0.96491900
H	3.98298900	-2.49530800	-1.83508400
C	5.80840200	-2.49486500	0.15643500
C	6.53217100	-2.36636800	1.50001100
H	7.58418400	-2.63473500	1.37333300
H	6.49809700	-1.34097900	1.88230600
H	6.10854400	-3.03781000	2.25368000
C	5.93932100	-3.94871700	-0.32912700
H	5.48144300	-4.09395200	-1.31159700
H	6.99648700	-4.21841900	-0.41165300
H	5.46374600	-4.63927600	0.37355500
C	6.48622400	-1.55217100	-0.85298800
H	7.54904700	-1.79848500	-0.93577600
H	6.04629700	-1.63899000	-1.85032400
H	6.39987300	-0.50973900	-0.53195800
O	-2.35956500	2.26833800	-1.12485800
C	-0.28713400	2.37882200	0.12451300
C	-0.84962100	3.20848900	1.09426400
C	1.02383600	1.91465600	0.27447400
C	-0.09456500	3.58622500	2.20297600
H	-1.86461700	3.57386900	0.96732000
C	1.77803000	2.30414200	1.37130400
H	1.44944100	1.26194900	-0.48422700
C	1.21712000	3.14118100	2.33959500
H	-0.53017900	4.23854500	2.95262400
H	2.80431800	1.96265900	1.46667700
H	1.80794600	3.45301200	3.19508100
C	1.48182300	3.68681400	-2.11554700
C	0.92871300	4.71885000	-1.35041300
C	2.87224400	3.54584100	-2.16926200
C	1.74975700	5.55632200	-0.60485000
H	-0.14831400	4.85944500	-1.34512400
C	3.69287200	4.37971900	-1.41758400
H	3.30794600	2.76402900	-2.78584500
C	3.13206800	5.38020000	-0.62709900

H	1.31070500	6.35081800	-0.01033000
H	4.77001100	4.25415400	-1.45437800
H	3.77183300	6.03413700	-0.04364500
C	0.63298800	2.74016100	-2.86399100
H	0.92012100	2.57682700	-3.90253000
C	-0.45117500	2.06778600	-2.44557100
H	-1.00794300	1.48343800	-3.17258900

I_7



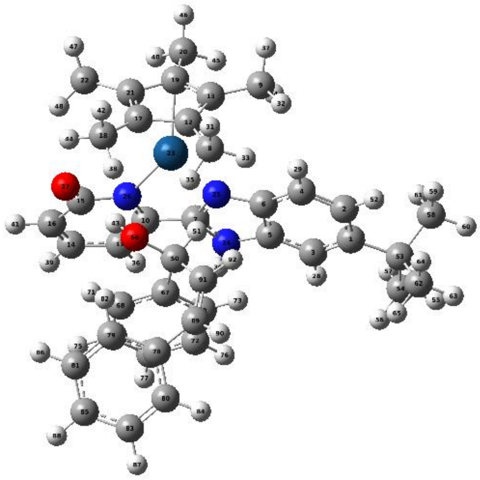
I_7	
SCF Done: E (RM062X)	**-2007.168149**
Thermal correction to Gibbs Free Energy	**0.694150**

C	4.99582900	-0.65305000	0.08177400
C	4.22050700	-0.98838400	-1.06127700
C	4.35638700	-0.45490600	1.29847500
C	2.85001400	-1.14452300	-1.02541100
C	2.96865700	-0.60966100	1.33636800
C	2.21393500	-0.96466400	0.20725600
C	0.82038600	-0.70096200	1.84340400
C	-1.84559600	-1.43651900	-3.51537900
C	0.59242400	-3.34156500	-2.61529100
C	-0.47798800	-0.54493100	2.48175100
C	-0.67244800	-0.37741100	3.83876900
C	-1.74208900	-2.21927400	-2.24494100
C	-0.63125800	-3.02412400	-1.81443400
C	-1.98464800	-0.21810800	4.29666900
C	-2.72653100	-0.30351900	2.01244100
C	-3.01543800	-0.16890800	3.38393700
C	-2.76738800	-2.32478700	-1.24936300
C	-4.15717500	-1.77987900	-1.38285400
C	-1.04342700	-3.75783100	-0.61419000
C	-0.17892700	-4.75016500	0.09877800
C	-2.33059700	-3.32482800	-0.27044800
C	-3.14947900	-3.73302400	0.91298600
Ir	-0.96507100	-1.43068900	-0.39005800

N	2.04983000	-0.45515000	2.36076000
N	0.88250900	-1.02987300	0.56988500
N	-1.48922700	-0.56530900	1.57677100
O	-3.71889400	-0.17463100	1.14994700
H	4.90487800	-0.18639000	2.19315500
H	2.27551600	-1.37749500	-1.91352500
H	2.24570100	-0.13213300	3.29572600
H	-2.24006800	-2.07320300	-4.31404100
H	0.84569100	-2.52504100	-3.29535100
H	-0.87289800	-1.05221700	-3.82827300
H	1.45227800	-3.53940400	-1.97083100
H	-2.52534000	-0.59175400	-3.38497300
H	0.16515700	-0.39358200	4.52636300
H	0.41479700	-4.23760900	-3.21980300
H	-4.14479500	-0.75177300	-1.75164800
H	-2.18550000	-0.10904700	5.35698000
H	-0.56735000	-4.97718400	1.09311600
H	-4.04566900	0.00116800	3.67111700
H	-4.72675500	-2.39342500	-2.08889700
H	-3.41586300	0.23561200	0.29594000
H	-4.68185600	-1.78845400	-0.42689300
H	0.84221400	-4.37391400	0.20923100
H	-0.12777700	-5.68778800	-0.46431900
H	-3.90190800	-4.47057700	0.61512900
H	-3.68096500	-2.87197900	1.32702800
H	-2.53429600	-4.17337600	1.69969400
C	-2.15985200	2.05688600	-1.07758900
H	-0.72962200	-0.03188400	-1.02845200
H	4.72877100	-1.12284800	-2.01036900
C	6.51217100	-0.51579100	-0.07322200
C	7.19278100	-0.13482200	1.24486300
H	8.27040600	-0.04536200	1.08483900
H	6.83429400	0.82853100	1.62192000
H	7.03614700	-0.89550400	2.01641000
C	7.09245500	-1.85842600	-0.54988800
H	6.67490900	-2.16408100	-1.51330900
H	8.17698400	-1.77379400	-0.66797000
H	6.88727600	-2.65052900	0.17627800
C	6.81923900	0.57706000	-1.11148900
H	7.90176100	0.68747300	-1.22592300
H	6.40476600	0.33526000	-2.09397600
H	6.40798900	1.54070300	-0.79609400
O	-3.16247900	1.34661900	-0.99625500
C	-1.37505700	2.37692000	0.15331000
C	-2.06062700	2.59584600	1.34912400
C	0.02253600	2.38753300	0.13585200
C	-1.35269700	2.83934300	2.52219700
H	-3.14760900	2.57745500	1.34841600
C	0.72836100	2.61404600	1.31163100
H	0.54946000	2.20804500	-0.79650800
C	0.04097600	2.84638000	2.50347000
H	-1.88632600	3.02711800	3.44838600
H	1.81409800	2.61945900	1.29439000
H	0.59116700	3.04504000	3.41862100

C	-0.62559100	4.72086100	-1.87114000
C	-1.49196100	5.22934000	-0.89604200
C	0.63945400	5.29994700	-2.02801100
C	-1.08087300	6.25913100	-0.05939300
H	-2.49680900	4.82578600	-0.81148500
C	1.05390500	6.32352200	-1.18406000
H	1.30463200	4.93060200	-2.80388200
C	0.19663900	6.79958800	-0.19424000
H	-1.76136400	6.64933200	0.68998000
H	2.04061600	6.75800200	-1.30504000
H	0.51569300	7.60677100	0.45682300
C	-1.01319300	3.60042000	-2.74081100
H	-0.71259200	3.69556500	-3.78396600
C	-1.70575700	2.49388800	-2.41440200
H	-2.00849900	1.81399900	-3.20604800

I$_8$



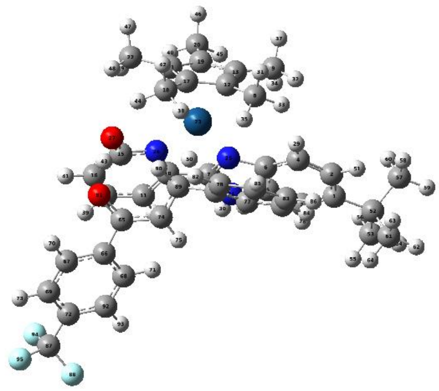
I$_8$	
SCF Done: E (RM062X)	-2007.147327
Thermal correction to Gibbs Free Energy	0.700076

C	4.83230600	1.39829100	0.01460800
C	4.37807500	0.54397800	-1.01915100
C	4.06455400	1.53753600	1.16056800
C	3.20590600	-0.18342100	-0.94193300
C	2.88020400	0.80917300	1.24518900
C	2.44565800	-0.06115200	0.23156300
C	0.91322900	-0.03856500	1.79920400
C	-0.32876800	-1.79382000	-3.26054500
C	2.18501700	-3.38139200	-1.89509200
C	-0.39369800	-0.28621800	2.38202100
C	-0.83053200	0.21278200	3.56910200
C	-0.34185100	-2.68926300	-2.06844900
C	0.76332000	-3.34097300	-1.44631400
C	-2.18368300	-0.04471000	3.93369700

C	-2.52776300	-1.15871000	1.77238800
C	-3.00233200	-0.70511800	3.07435000
C	-1.56693000	-3.07590000	-1.37566000
C	-2.94877800	-2.76055400	-1.85158400
C	0.25536400	-4.02749800	-0.28484600
C	1.06965700	-4.82792400	0.67476000
C	-1.19219200	-3.89901700	-0.27466000
C	-2.11461100	-4.53045100	0.71339900
Ir	-0.20817600	-1.98011100	-0.02413800
N	1.89408900	0.77517600	2.22329000
N	1.21637700	-0.59661700	0.62625700
N	-1.16594100	-1.03498100	1.53345200
O	-3.27402600	-1.60933000	0.88869200
H	4.36416200	2.19441700	1.96925300
H	2.87407400	-0.80191600	-1.76622900
H	1.82189500	1.39609500	3.01578600
H	-0.57188200	-2.37153500	-4.16092400
H	2.34608700	-2.71897700	-2.74614000
H	0.65245100	-1.33077700	-3.40109700
H	2.87378100	-3.10283000	-1.09648200
H	-1.08340100	-1.00825700	-3.14466300
H	-0.18306000	0.80013300	4.20986500
H	2.43178400	-4.39931800	-2.21475900
H	-3.00854600	-1.75063300	-2.23957100
H	-2.55928700	0.31558300	4.88684000
H	0.60378300	-4.86055600	1.66128600
H	-4.04789900	-0.88755200	3.29365600
H	-3.19081900	-3.45859900	-2.65817400
H	-2.57462900	-0.25098200	-0.59275600
H	-3.68516900	-2.86756500	-1.04597500
H	2.07362100	-4.41336700	0.77761700
H	1.15490500	-5.85567200	0.30447700
H	-2.39460500	-5.53291600	0.37154500
H	-3.01644400	-3.92401400	0.82807600
H	-1.63439400	-4.62541400	1.68757900
C	-1.24227800	1.08711600	-1.26129100
H	-0.36158300	0.41891100	-1.17328000
H	4.97490300	0.46144900	-1.92113000
C	6.15127500	2.14969400	-0.17578500
C	6.48595900	3.02245500	1.03234200
H	7.43500200	3.53462500	0.85539800
H	5.72156500	3.78899400	1.19778900
H	6.59612300	2.42768100	1.94575600
C	7.28637600	1.13092200	-0.37212700
H	7.12421500	0.51203200	-1.26014400
H	8.23862200	1.65372600	-0.50011100
H	7.37507500	0.46861300	0.49420500
C	6.05115500	3.05678500	-1.41643100
H	6.98931300	3.60393800	-1.55216000
H	5.86780600	2.48465800	-2.32957000
H	5.24304500	3.78573500	-1.30656700
O	-2.40344900	0.27849700	-1.40310700
C	-1.22063600	1.95747600	-0.01639600
C	-2.32386800	2.06160100	0.83048100

C	-0.04566900	2.64637100	0.30631500
C	-2.25880300	2.84806400	1.97873000
H	-3.24851500	1.54420800	0.58051600
C	0.02171500	3.43206000	1.45244100
H	0.81674900	2.57217300	-0.35552400
C	-1.08708200	3.53427400	2.29489100
H	-3.12926700	2.93169500	2.62001000
H	0.93336900	3.97984400	1.68007600
H	-1.04469500	4.16151500	3.17936300
C	-2.67030600	3.66705600	-2.01041100
C	-3.77159800	2.95000900	-1.52405000
C	-2.57662100	5.03832800	-1.75800000
C	-4.74347300	3.59376500	-0.77684900
H	-3.84345600	1.88674200	-1.74522800
C	-3.54171300	5.67671700	-1.00351300
H	-1.73674900	5.60506400	-2.14797900
C	-4.62664400	4.95721300	-0.50925500
H	-5.59730200	3.03342200	-0.41147300
H	-3.45477300	6.74195600	-0.80370800
H	-5.38761000	5.46897300	0.07195700
C	-1.63340800	3.02289200	-2.82473100
H	-1.33996200	3.54257100	-3.73868900
C	-1.03062200	1.88134100	-2.53172600
H	-0.29606000	1.48900800	-3.22924000

TS$_{3\text{-}CF3}$



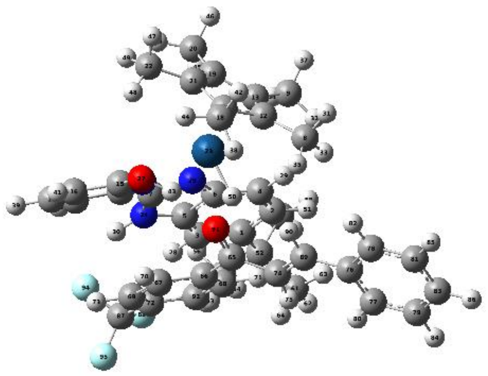
TS$_{3\text{-}CF3}$	
SCF Done: E (RM062X)	-2344.075659
Thermal correction to Gibbs Free Energy	0.691664

C	-3.76290300	3.89035800	-0.37766900
C	-4.11898500	2.72546600	0.35642500
C	-2.64675300	3.85687400	-1.20365300
C	-3.41749200	1.54042900	0.27555600
C	-1.92966600	2.66021900	-1.27946400
C	-2.30954100	1.50711300	-0.57800100
C	-0.48184300	1.02826700	-1.65100900

C	-3.38808000	-2.35376900	1.86008000
C	-4.48576000	-1.37606000	-1.03187900
C	0.70308500	0.23787300	-1.95795700
C	1.85502900	0.72311300	-2.54193100
C	-2.79356500	-2.65238100	0.52023700
C	-3.29247000	-2.23759800	-0.76047100
C	2.98260200	-0.10970800	-2.55581700
C	1.71511900	-1.77157500	-1.34083900
C	2.91962700	-1.34280300	-1.94723100
C	-1.66412200	-3.54213700	0.27510300
C	-0.87042000	-4.25101200	1.32380900
C	-2.47982300	-2.82260900	-1.79034200
C	-2.70420300	-2.71149500	-3.26397100
C	-1.47617600	-3.63868700	-1.13834300
C	-0.48711100	-4.49480800	-1.86189000
Ir	-1.20230500	-1.55907400	-0.48486200
N	-0.76521400	2.31907700	-1.95076000
N	-1.39265800	0.50793300	-0.84639400
N	0.60798300	-1.01207200	-1.43215100
O	1.65397100	-2.86345400	-0.62211300
H	-2.32864300	4.72691900	-1.76513200
H	-3.67908100	0.67117200	0.86928200
H	-0.22296000	2.92283700	-2.55020600
H	-4.02036600	-3.18617500	2.18598200
H	-4.92881400	-0.99523500	-0.11168200
H	-4.00536500	-1.45354500	1.83169900
H	-4.23116600	-0.52505700	-1.66935900
H	-2.61264000	-2.19459600	2.61271300
H	1.89911600	1.73054100	-2.93921800
H	-5.24557900	-1.97073900	-1.54838300
H	-0.90422000	-3.70237700	2.26930600
H	3.91017000	0.23560400	-2.99972800
H	-1.76156300	-2.77002200	-3.81201000
H	3.78219800	-1.99404700	-1.87194800
H	-1.28050900	-5.25039100	1.49998100
H	2.35891200	-2.68846400	0.20879300
H	0.17216900	-4.34918200	1.01270700
H	-3.19175800	-1.76799000	-3.51878800
H	-3.34616400	-3.52781000	-3.61320100
H	-1.01519100	-5.33908000	-2.31716500
H	0.28039500	-4.87487600	-1.19049300
H	0.01203400	-3.93856000	-2.65950300
H	-0.20615700	-1.18945800	0.84213700
H	-4.97856500	2.77207200	1.01717500
C	-4.61514200	5.15046700	-0.21269900
C	-4.10001100	6.30868200	-1.07179000
H	-4.74228000	7.18114200	-0.92698300
H	-3.08229200	6.59932300	-0.79206400
H	-4.11600400	6.06005500	-2.13783000
C	-6.06275700	4.84038200	-0.63134800
H	-6.50457500	4.04911300	-0.01930600
H	-6.68150900	5.73514200	-0.51475500
H	-6.10751200	4.52661200	-1.67843000
C	-4.58710500	5.58879300	1.26202700

H	-5.18958300	6.49288900	1.39118900
H	-4.99539600	4.82071500	1.92469000
H	-3.56508800	5.80941500	1.58418800
C	2.99178900	-0.86538400	1.20168800
C	4.17510600	0.00258900	0.92527200
C	5.44446700	-0.58301500	0.94568100
C	4.04763400	1.35534300	0.58872700
C	6.57278600	0.17367100	0.65618900
H	5.52500100	-1.63493600	1.19609200
H	3.06727900	1.81730600	0.53374900
C	6.43152600	1.51890000	0.32638600
H	7.56109400	-0.27180900	0.69052800
C	1.77186700	-0.28336400	1.59988200
H	1.71240100	0.78701600	1.75613600
C	-0.35303800	-0.59962400	2.92152000
C	-1.07710700	0.57131600	2.68147400
C	-0.59583300	-1.32667700	4.08876100
C	-2.03541700	1.00568300	3.58806100
H	-0.89971100	1.12589600	1.76289000
C	-1.55147500	-0.88512900	5.00437500
H	-0.02756000	-2.23164300	4.28831600
C	-2.27573500	0.27610900	4.75325900
H	-2.59724500	1.91204000	3.38281600
H	-1.72956200	-1.45184900	5.91226800
H	-3.02299200	0.61491300	5.46300800
C	7.63758400	2.33215900	-0.05695400
F	7.50495800	3.61024200	0.31958100
C	0.66565700	-1.08483900	1.94459900
H	0.89012300	-2.15153000	2.00632100
O	3.16913700	-2.12499500	1.07895300
C	5.17218700	2.11219800	0.28854400
H	5.07987300	3.16216100	0.03150100
F	7.81426600	2.33064000	-1.38769100
F	8.75521900	1.85003500	0.49490500

$I_{5\text{-}CF3}$



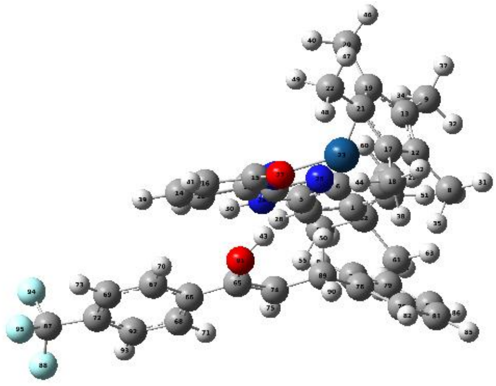
$I_{5\text{-}CF3}$

SCF Done: E (RM062X)	-2344.098134
Thermal correction to Gibbs Free Energy	0.701082

C	4.09229400	2.44657300	-1.56869300
C	2.83258600	2.47712700	-2.22784200
C	4.37215900	1.40839700	-0.69033600
C	1.86051100	1.51449500	-2.04611200
C	3.38943600	0.43308400	-0.50460800
C	2.15244500	0.46469100	-1.16820900
C	2.11482200	-1.23180900	0.17479500
C	-3.16528300	0.20981800	-2.25456500
C	-0.53309000	-0.18105900	-4.09452300
C	1.49684700	-2.26950600	0.98668600
C	2.17348600	-3.09233200	1.86458400
C	-2.27118300	-0.98934000	-2.30627000
C	-1.07416100	-1.14538400	-3.08605600
C	1.41849700	-3.96906000	2.65137300
C	-0.57073300	-3.05283500	1.66249200
C	0.04288900	-3.94095800	2.56559200
C	-2.48020800	-2.21207200	-1.58274300
C	-3.70078600	-2.53876900	-0.77638400
C	-0.62750400	-2.53527200	-2.96116900
C	0.55352500	-3.10559500	-3.68224300
C	-1.47467500	-3.17251600	-2.04326100
C	-1.37534400	-4.57413700	-1.52993800
Ir	-0.59898500	-1.29301900	-0.97618600
N	3.33931200	-0.67053100	0.32709600
N	1.39188100	-0.60158900	-0.72950100
N	0.14619200	-2.28242900	0.83781200
O	-1.89231500	-2.99330600	1.63981200
H	5.30927600	1.35225400	-0.14991200
H	0.89708500	1.57047700	-2.53940300
H	4.00370600	-0.90245300	1.05251900
H	-3.98572100	0.09565200	-2.97036600
H	-0.85873900	0.83978000	-3.88395000
H	-2.61987200	1.12326600	-2.49849800
H	0.55935400	-0.19954900	-4.11925600
H	-3.58962900	0.32973800	-1.25495800
H	3.25348400	-3.05814000	1.93641600
H	-0.89557700	-0.44776300	-5.09297200
H	-3.97888900	-1.70538500	-0.12584300
H	1.90983400	-4.64496600	3.34295300
H	0.86932800	-4.05382700	-3.24400000
H	-0.59563200	-4.55872300	3.18465500
H	-4.54192800	-2.75089500	-1.44481000
H	-2.20560600	-2.07238100	1.45275900
H	-3.53875700	-3.41544300	-0.14768100
H	1.40336900	-2.41802700	-3.65219800
H	0.31041800	-3.28666700	-4.73441100
H	-2.09758100	-5.21799100	-2.04224100
H	-1.60553900	-4.60653800	-0.46144700

H	-0.37853000	-4.99101500	-1.68413500
H	-0.94756100	-0.00333500	-0.18854700
H	2.62098600	3.30172000	-2.90080300
C	5.09260400	3.57181500	-1.84179300
C	6.39327200	3.38703000	-1.05514900
H	7.07624800	4.20898400	-1.28471300
H	6.21803700	3.39548900	0.02547100
H	6.89833400	2.45329200	-1.32219900
C	5.43055000	3.59433000	-3.34244400
H	4.54457800	3.77543500	-3.95740800
H	6.14864700	4.39362800	-3.54920700
H	5.87438300	2.64502200	-3.65646700
C	4.46547400	4.91626900	-1.43472700
H	5.17426700	5.72877700	-1.62087400
H	3.55607300	5.13190400	-2.00253300
H	4.21179200	4.92115700	-0.37026000
C	-2.32851400	0.60054100	1.89357600
C	-0.90010500	0.63976800	2.34520100
C	-0.45221700	-0.30574700	3.27265700
C	0.00038500	1.54389900	1.77847400
C	0.89031900	-0.35062700	3.62454200
H	-1.16452800	-1.00379600	3.70359900
H	-0.34147800	2.26109300	1.03851300
C	1.78784200	0.53035500	3.01806900
H	1.24867200	-1.07893100	4.34617300
C	-3.00011200	1.87390900	1.61783800
H	-2.44810400	2.78847200	1.80496100
C	-5.11140600	3.04081100	0.89601800
C	-4.64702600	4.36006300	1.02025600
C	-6.42850300	2.82488400	0.46757800
C	-5.47994500	5.42747800	0.72289700
H	-3.63222200	4.55206500	1.35395200
C	-7.26331200	3.89520000	0.16940600
H	-6.79593500	1.80665600	0.37344700
C	-6.78944100	5.19784900	0.29665500
H	-5.11295600	6.44314300	0.82450100
H	-8.28115200	3.71426700	-0.15873000
H	-7.43806000	6.03648900	0.06611000
C	3.24378600	0.42723600	3.36915400
F	4.01201500	1.19327500	2.58080700
C	-4.28036300	1.88081600	1.19628200
H	-4.75329200	0.90602100	1.07193800
O	-2.89554700	-0.48456500	1.76267000
C	1.35259500	1.47937800	2.09771500
H	2.06302400	2.15212800	1.62788200
F	3.68948800	-0.84821800	3.20531700
F	3.49015700	0.75309900	4.63408600

I$_{6\text{-CF3}}$



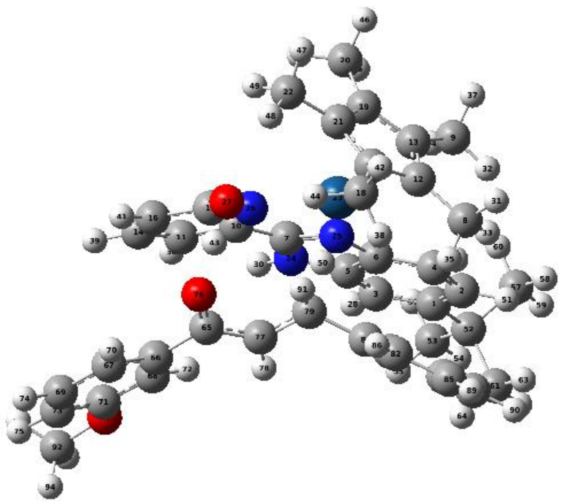
I6-CF3	
SCF Done: E (RM062X)	-2344.116357
Thermal correction to Gibbs Free Energy	0.695151

C	-3.89979100	3.98528900	-0.20320200
C	-4.45332300	2.73411100	0.17313300
C	-2.60247400	4.02619100	-0.69998500
C	-3.77326600	1.53783600	0.04595300
C	-1.91509300	2.81835200	-0.82094900
C	-2.48254200	1.58280700	-0.48438200
C	-0.43040800	1.20385800	-1.12823300
C	-3.42719100	-2.34577700	1.74575200
C	-4.71758900	-1.52673800	-1.13009400
C	0.76987700	0.41074900	-1.34309100
C	1.96893900	0.91260200	-1.75468500
C	-2.89514200	-2.65752800	0.38853300
C	-3.44475600	-2.26586500	-0.86119400
C	3.04986700	0.00073600	-1.91642700
C	1.61641600	-1.79844300	-1.05769600
C	2.87229800	-1.30841100	-1.60538700
C	-1.71352500	-3.49052400	0.13024300
C	-0.90558900	-4.18001800	1.17608300
C	-2.56054300	-2.76280400	-1.89283800
C	-2.75626500	-2.57989900	-3.35941800
C	-1.53599600	-3.58498600	-1.27493700
C	-0.54237100	-4.40489700	-2.03004000
Ir	-1.39899700	-1.48396700	-0.66936600
N	-0.61577500	2.53418400	-1.22526200
N	-1.53465300	0.59374300	-0.70790700
N	0.54939500	-0.91385700	-1.04530000
O	1.49360800	-2.94398700	-0.59914000
H	-2.12874700	4.95978800	-0.97838500
H	-4.20505000	0.60082300	0.37464100
H	0.07968800	3.20612000	-1.51551300
H	-4.03501800	-3.18407800	2.10315500
H	-5.21923400	-1.24905800	-0.20228800
H	-4.04727400	-1.44752900	1.73712700
H	-4.55198500	-0.62361300	-1.72324400

H	-2.61450000	-2.18307400	2.45738700
H	2.09638100	1.96777700	-1.96666200
H	-5.39562900	-2.17884800	-1.68930100
H	-0.89673100	-3.60492300	2.10538800
H	4.01420100	0.36140000	-2.25986200
H	-1.80297300	-2.61002400	-3.88984300
H	3.67663800	-2.03146200	-1.67155200
H	-1.35240000	-5.15828000	1.38418300
H	2.92141200	-2.82721900	0.81953600
H	0.12019600	-4.31768300	0.83208400
H	-3.25105600	-1.63121700	-3.57665300
H	-3.38546600	-3.39042100	-3.74401100
H	-1.06985200	-5.22908200	-2.52165800
H	0.22482100	-4.80396600	-1.37106100
H	-0.04014100	-3.81191600	-2.79789800
H	0.91681900	-2.24027700	1.47943500
H	-5.45589200	2.71434800	0.58790100
C	-4.74568600	5.24849300	-0.03059600
C	-4.00559700	6.50359400	-0.50144800
H	-4.65117800	7.37559000	-0.36932800
H	-3.09354000	6.67946500	0.07800500
H	-3.74375000	6.44490400	-1.56286900
C	-6.03673400	5.10745400	-0.85534300
H	-6.63883700	4.25445100	-0.53005000
H	-6.64819000	6.00759600	-0.74277400
H	-5.80975100	4.97864300	-1.91780200
C	-5.09994200	5.41915500	1.45672300
H	-5.70673300	6.31938300	1.59238500
H	-5.67441700	4.57050600	1.83856900
H	-4.19588900	5.52032000	2.06454000
C	3.45939000	-1.06944300	1.40916300
C	4.55797800	-0.14884900	1.02672700
C	5.66821000	-0.66093500	0.34592400
C	4.49796500	1.22907900	1.27454900
C	6.67867800	0.18239500	-0.10275400
H	5.72992700	-1.72831800	0.17182100
H	3.66768800	1.65303400	1.82856200
C	6.58787100	1.55074000	0.12539400
H	7.54045400	-0.22096200	-0.62393200
C	2.30291700	-0.69270900	1.97759100
H	2.13463000	0.35403500	2.20092400
C	0.01226300	-1.06407300	2.99959100
C	-0.59429100	0.05667200	2.42093000
C	-0.56267100	-1.60603000	4.15170700
C	-1.74454600	0.61842300	2.97076200
H	-0.13637700	0.50692600	1.54339700
C	-1.71070000	-1.04451800	4.71157100
H	-0.09442000	-2.46409300	4.62715100
C	-2.30610900	0.06788300	4.12198000
H	-2.19085500	1.49683100	2.51270900
H	-2.13135600	-1.47070100	5.61669900
H	-3.19210800	0.51124300	4.56442000
C	7.62843200	2.47964200	-0.43004900
F	7.80400900	3.55147800	0.35311000

C	1.23894000	-1.68251400	2.37223600
H	1.66284500	-2.43250200	3.05371600
O	3.73111700	-2.37015600	1.10320900
C	5.50108800	2.07388100	0.82337400
H	5.45330200	3.13938300	1.02222900
F	7.26861700	2.93655700	-1.64279900
F	8.81166000	1.87272700	-0.57413300

TS$_{3\text{-OMe}}$



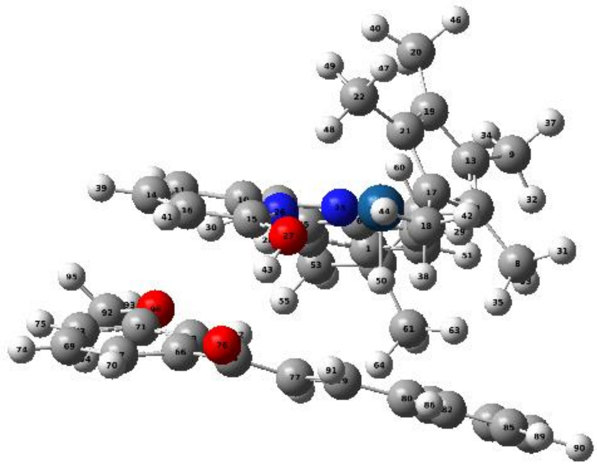
TS$_{3\text{-OMe}}$	
SCF Done: E (RM062X)	-2121.594618
Thermal correction to Gibbs Free Energy	0.720483

C	-4.20190500	3.03533200	-0.32051800
C	-4.28117800	1.79824900	0.37602200
C	-3.10503200	3.28729500	-1.13428000
C	-3.32164100	0.81251700	0.27072900
C	-2.12851300	2.29316400	-1.23629400
C	-2.23357200	1.06362900	-0.57082800
C	-0.33844900	1.05378700	-1.63326300
C	-2.38481700	-2.92809800	1.82422400
C	-3.66671500	-2.26511500	-1.08149900
C	0.99968700	0.56942500	-1.94469800
C	2.00753500	1.32713100	-2.50334200
C	-1.72744800	-3.08537500	0.48920200
C	-2.30200500	-2.81174900	-0.79834900
C	3.29975600	0.78429700	-2.52221700
C	2.45344100	-1.15724000	-1.35358800
C	3.52545100	-0.44238700	-1.94159900
C	-0.41782400	-3.68312500	0.25685000
C	0.51771000	-4.17226600	1.31389200
C	-1.36546900	-3.19170700	-1.81856200

C	-1.59742300	-3.14466400	-3.29441100
C	-0.20158100	-3.74188000	-1.15398700
C	0.96680900	-4.34995500	-1.86083200
Ir	-0.43434000	-1.65105200	-0.51645900
N	-0.91307200	2.25086700	-1.90287400
N	-1.10868100	0.31279400	-0.85496600
N	1.19663600	-0.68072800	-1.44700100
O	2.65317400	-2.23709900	-0.64719100
H	-2.99478800	4.22489100	-1.66537300
H	-3.37293000	-0.11083100	0.83797300
H	-0.51443000	2.98716100	-2.46558500
H	-2.80192000	-3.88495700	2.15489700
H	-4.20369200	-2.02415500	-0.16410300
H	-3.19931200	-2.20177500	1.78427600
H	-3.62470800	-1.36580600	-1.70180600
H	-1.67476600	-2.58224500	2.57935800
H	1.81672900	2.32869900	-2.87100500
H	-4.24828000	-3.01993500	-1.61991500
H	0.33459400	-3.65371400	2.25898800
H	4.12307200	1.35032900	-2.94434400
H	-0.66053500	-2.99413000	-3.83464000
H	4.51807900	-0.86865200	-1.85986300
H	0.37357700	-5.24390500	1.48347500
H	3.30956800	-1.89884100	0.19697600
H	1.55471100	-4.00074100	1.01484900
H	-2.28050300	-2.33540300	-3.56069600
H	-2.03728100	-4.08625700	-3.64126400
H	0.66797300	-5.32230300	-2.26632200
H	1.81356800	-4.48571100	-1.19091500
H	1.29640500	-3.72314100	-2.69305200
H	0.45832400	-1.05293400	0.80851800
H	-5.13124200	1.62349200	1.02753800
C	-5.32455800	4.05755100	-0.12990600
C	-5.08747900	5.33122400	-0.94623000
H	-5.91501700	6.02636500	-0.78320800
H	-4.16624900	5.84022600	-0.64498300
H	-5.03981200	5.12093000	-2.01953800
C	-6.65704700	3.43312800	-0.57879000
H	-6.90694300	2.54190000	0.00345200
H	-7.46826900	4.15522700	-0.44638700
H	-6.61967800	3.15011700	-1.63494000
C	-5.41074800	4.44185500	1.35759600
H	-6.20629100	5.17820400	1.50516900
H	-5.63633900	3.57852100	1.98980000
H	-4.46967100	4.88046000	1.70255600
C	3.48928500	0.00017500	1.17978700
C	4.43301400	1.12221800	0.91433800
C	5.80879400	0.88151100	1.01742300
C	3.97545900	2.37288100	0.50548700
C	6.70115700	1.90649500	0.74324700
H	6.14824900	-0.10254400	1.31822000
C	4.88130500	3.39493700	0.21135400
H	2.91860500	2.58114100	0.37454600
C	6.25263800	3.16562700	0.33997200

H	7.76817200	1.73430800	0.83943100
H	6.97211700	3.94716600	0.12808800
O	3.95724300	-1.18568800	1.05416200
C	2.16476400	0.27598400	1.57560600
H	1.85818800	1.30299400	1.73579600
C	1.27992300	-0.76882200	1.90629900
C	0.18500500	-0.56974300	2.90165200
C	-0.82434100	0.37498000	2.69723100
C	0.16248200	-1.35565000	4.05611400
C	-1.84738700	0.52326900	3.62594200
H	-0.81390200	0.97666800	1.79135600
C	-0.85885900	-1.20030000	4.99302000
H	0.95221800	-2.08272100	4.22672300
C	-1.86799000	-0.26721300	4.77618600
H	-2.63043700	1.25495000	3.45060600
H	-0.86480600	-1.81159500	5.88928400
H	-2.66590700	-0.15161300	5.50197100
H	1.75454900	-1.75122500	1.95004300
C	5.20562200	5.65261600	-0.42796100
H	4.57681600	6.49734900	-0.70608900
H	5.77013300	5.90279700	0.47725100
H	5.90685900	5.43851100	-1.24315700
O	4.33058900	4.56519800	-0.20182500

I5-OMe



I5-OMe	
SCF Done: E (RM062X)	**-2121.618148**
Thermal correction to Gibbs Free Energy	**0.732104**

C	-4.86614800	-1.56799800	0.34764800
C	-3.83087900	-2.53163600	0.48709800
C	-4.56217700	-0.32315100	-0.18573900
C	-2.52630800	-2.30007300	0.10253200

C	-3.24176000	-0.08472300	-0.57318300
C	-2.23107200	-1.05177500	-0.45497600
C	-1.31642200	0.73928000	-1.24908000
C	2.37767400	-3.40067200	0.93240800
C	0.12903800	-4.18933400	-1.22876700
C	-0.23381500	1.64907100	-1.58682000
C	-0.41167500	2.92366200	-2.09440700
C	2.18487900	-2.78925700	-0.41833500
C	1.15660100	-3.11036400	-1.36534700
C	0.71004500	3.74500600	-2.20646100
C	2.03215300	1.95820300	-1.29192800
C	1.93678900	3.26686100	-1.78936700
C	3.03744500	-1.79942600	-1.02114400
C	4.32325300	-1.30611600	-0.43248900
C	1.45098400	-2.41974000	-2.61753300
C	0.64428800	-2.55947100	-3.87043100
C	2.58728400	-1.62081700	-2.40026700
C	3.23126900	-0.69548300	-3.38424500
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N	-2.62929700	1.04261800	-1.09489700
N	-1.04189200	-0.49992200	-0.89538600
N	0.97505900	1.14732800	-1.22940500
O	3.19073200	1.46434600	-0.83656300
H	-5.31494400	0.44694300	-0.30196100
H	-1.74799300	-3.03928000	0.24311500
H	-2.97651200	1.99115500	-0.99710000
H	2.97867000	-4.31228100	0.84573400
H	-0.05609600	-4.43344100	-0.18069600
H	1.42229600	-3.65822900	1.39431200
H	-0.81705100	-3.90666500	-1.69713100
H	2.89387400	-2.70946000	1.60187800
H	-1.40023900	3.27039200	-2.37355400
H	0.48783400	-5.09862600	-1.72302900
H	4.18595100	-1.03090900	0.61671700
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H	-0.42703900	-2.51937600	-3.65473700
H	0.84965600	-3.51893500	-4.35692600
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H	0.84744100	-0.69480500	0.70836500
H	-4.07548400	-3.49458900	0.92343000
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H	-7.34924000	-0.52441100	-0.48030600
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H	-6.77812500	-2.94406600	-1.07177900
C	-6.26082300	-2.27988700	2.30030800
H	-7.26840200	-2.54639000	2.63374800
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C	1.80700500	2.98875800	1.52687300
C	0.62816800	3.86100100	1.21654500
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C	-0.17855700	6.04402300	0.59519700
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H	-0.87521100	2.29060300	1.23741600
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C	2.62574900	-0.37019500	3.17821400
C	1.43366700	-1.03779500	3.50094800
C	3.84787000	-0.95936400	3.53322600
C	1.46898000	-2.25200100	4.17178100
H	0.47809200	-0.61141300	3.21215200
C	3.88263400	-2.17683200	4.20533000
H	4.77447600	-0.44694700	3.28750500
C	2.69206700	-2.82378400	4.52681000
H	0.54199000	-2.75895300	4.41884200
H	4.83500200	-2.61693700	4.48105900
H	2.71490700	-3.77216400	5.05356700
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C	-4.04791200	4.41235900	0.33432500
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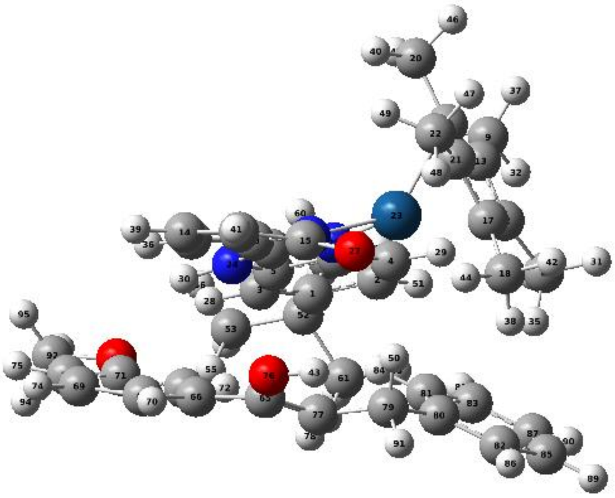
H	-4.10106500	5.08967700	1.19203100
H	-4.03913300	4.99628900	-0.59262700
O	-2.90756500	3.56893600	0.42920700

$I_{6\text{-OMe}}$



$I_{6\text{-OMe}}$	
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Thermal correction to Gibbs Free Energy	**0.725736**

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C	2.37390100	2.47271400	-0.53758500
C	2.09834800	3.81433700	-1.04420800
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O	3.39399400	2.18667700	0.09141100
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H	3.81104100	-1.88913300	-4.06183100
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C	-0.17426000	-1.31631900	2.58291500
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C	-0.48326200	-2.63285500	2.91684900

H	-0.73446000	-0.81626500	1.79722400
C	1.23550800	-2.60683800	4.60051600
H	2.30092500	-0.75214500	4.82783000
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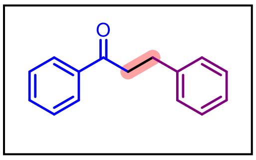
H	1.63445700	1.27806000	3.81567600
C	-5.40735200	3.29349700	-0.81444800
H	-6.09004000	2.48326200	-1.06816200
H	-5.88530100	3.96215600	-0.09199600
H	-5.15620600	3.85535600	-1.72081400
O	-4.25696800	2.68309000	-0.24785800

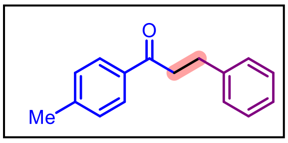
9. Spectral Data for the Transfer Hydrogenation of α,β-Unsaturated Ketones and Imines

1,3-diphenylpropan-1-one (2):[9]



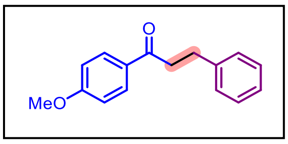
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 92% (96.7 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 77.95 (d, $J_{H,H}$ = 7.7 Hz, 2H), 7.55 (t, $J_{H,H}$ = 7.4 Hz, 1H), 7.44 (t, $J_{H,H}$ = 7.6 Hz, 2H), 7.25 (m, 5H), 3.30 (t, $J_{H,H}$ = 7.7 Hz, 2H), 3.07 (t, $J_{H,H}$ = 7.7 Hz, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 199.3, 141.4, 137.0, 133.1, 128.7, 128.6, 128.5, 128.1, 126.2, 40.5, 30.2.

3-phenyl-1-(p-tolyl)propan-1-one (3):[10]



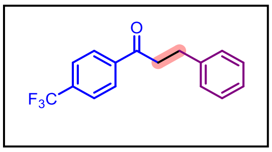
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 84% (94.2 mg) isolated yield; white solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.94 (dd, $J_{H,H}$ = 8.4, 1.3 Hz, 2H), 7.54 (t, $J_{H,H}$ = 7.4 Hz, 1H), 7.44 (t, $J_{H,H}$ = 7.8 Hz, 2H), 7.16 – 7.06 (m, 4H), 3.27 (t, $J_{H,H}$ = 7.3 Hz, 2H), 3.02 (t, $J_{H,H}$ = 7.9 Hz, 2H), 2.31 (s, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 199.4, 138.2, 136.9, 135.7, 133.1, 129.3, 128.7, 128.4, 128.1, 40.7, 29.8, 21.1.

1-(4-methoxyphenyl)-3-phenylpropan-1-one (4):[10]



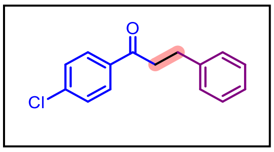
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (96.1 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.92 (d, $J_{H,H}$ = 8.6 Hz, 2H), 7.32-7.15 (m, 5H), 6.90 (d, $J_{H,H}$ = 8.6 Hz, 2H), 3.84 (s, 3H), 3.23 (t, $J_{H,H}$ = 7.9 Hz, 2H), 3.04 (t, $J_{H,H}$ = 7.7 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 197.9, 163.5, 141.6, 130.4, 130.1, 128.7, 128.6, 128.5, 126.2, 113.8, 55.5, 40.2, 30.4.

3-phenyl-1-(4-(trifluoromethyl)phenyl)propan-1-one (5):[11]



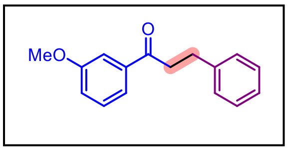
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 95% (132.2 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.04 (d, $J_{H,H}$ = 8.1 Hz, 2H), 7.71 (d, $J_{H,H}$ = 8.4 Hz, 2H), 7.36 – 7.17 (m, 5H), 3.32 (t, $J_{H,H}$ = 7.6 Hz, 2H), 3.09 (t, $J_{H,H}$ = 7.6 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 198.2, 140.9, 139.6, 134.9 (q, $J_{C,F}$ = 32.0 Hz), 128.7, 128.5, 128.4, 126.3, 125.7 (d, $J_{C,F}$ = 5.0 Hz), 125.0 (d, $J_{C,F}$ = 271.0 Hz), 40.8, 30.0.

1-(4-chlorophenyl)-3-phenylpropan-1-one (6):[12]



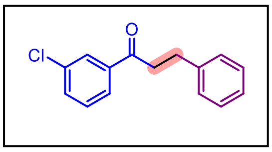
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 90% (110.1 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.87 (d, $J_{H,H}$ = 8.5 Hz, 2H), 7.41 (d, $J_{H,H}$ = 8.5 Hz, 2H), 7.32 – 7.26 (m, 2H), 7.25 – 7.18 (m, 3H), 3.26 (t, $J_{H,H}$ = 7.7 Hz, 2H), 3.05 (t, $J_{H,H}$ = 7.7 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 198.0, 141.1, 139.6, 135.3, 129.5, 129.0, 128.6, 128.5, 126.3, 40.5, 30.1.

1-(3-methoxyphenyl)-3-phenylpropan-1-one (7):[13]



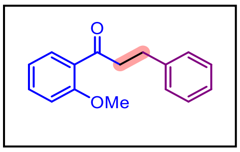
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 85% (102.1 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.55 – 7.48 (m, 2H), 7.36 – 7.19 (m, 6H), 7.09 (dd, $J_{H,H}$ = 8.2, 2.7 Hz, 1H), 3.83 (s, 3H), 3.28 (t, $J_{H,H}$ = 8.1 Hz, 2H), 3.06 (t, $J_{H,H}$ = 7.6 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 199.0, 159.8, 141.3, 138.2, 129.6, 128.5, 128.4, 126.1, 120.7, 119.5, 112.3, 55.4, 40.5, 30.2.

1-(3-chlorophenyl)-3-phenylpropan-1-one (8):[14]



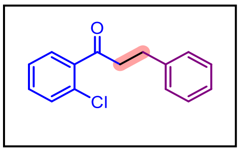
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 91% (111.4 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.90 (s, 1H), 7.80 (d, $J_{H,H}$ = 7.6 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.37 (t, $J_{H,H}$ = 7.9 Hz, 1H), 7.31 – 7.18 (m, 5H), 3.26 (t, $J_{H,H}$ = 7.7 Hz, 2H), 3.05 (t, $J_{H,H}$ = 7.6 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 197.9, 141.0, 138.4, 135.0, 133.0, 130.0, 128.6, 128.5, 128.2, 126.3, 126.1, 40.6, 30.0.

1-(2-methoxyphenyl)-3-phenylpropan-1-one (9):[15]



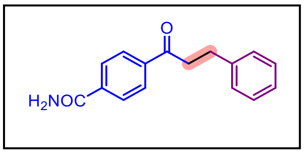
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (96.1 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.69 (dd, $J_{H,H}$ = 7.8, 1.8 Hz, 1H), 7.45 (td, $J_{H,H}$ = 7.9, 2.0 Hz, 1H), 7.30 – 7.17 (m, 5H), 7.01 – 6.93 (m, 2H), 3.87 (s, 3H), 3.30 (t, $J_{H,H}$ = 8.4 Hz, 2H), 3.02 (t, $J_{H,H}$ = 7.8 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 201.8, 158.6, 141.8, 133.5, 130.4, 128.5, 128.4, 128.3, 125.9, 120.7, 111.5, 55.5, 45.5, 30.5.

1-(2-chlorophenyl)-3-phenylpropan-1-one (10):[15]



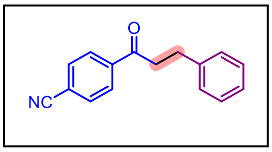
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 84% (102.8 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.39 – 7.32 (m, 3H), 7.29 – 7.23 (m, 3H), 7.22 – 7.14 (m, 3H), 3.25 (t, $J_{H,H}$ = 8.3 Hz, 2H), 3.03 (t, $J_{H,H}$ = 7.7 Hz, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 202.6, 140.8, 139.5, 131.8, 131.0, 130.6, 129.0, 128.6, 128.5, 127.0, 126.3, 44.6, 30.3.

4-(3-phenylpropanoyl)benzamide (11):[16]



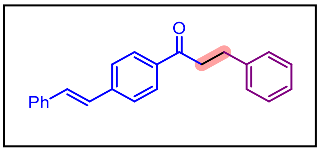
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 81% (102.6 mg) isolated yield; white solid. **^{1}H NMR** (500 MHz, DMSO-d_6): δ = 8.14 (s, 1H), 8.03 (d, $J_{H,H}$ = 8.4 Hz, 2H), 7.96 (d, $J_{H,H}$ = 8.3 Hz, 2H), 7.54 (s, 1H), 7.27 (d, $J_{H,H}$ = 4.5 Hz, 4H), 7.23 – 7.10 (m, 1H), 3.38 (t, $J_{H,H}$ = 7.6 Hz, 2H), 2.94 (t, $J_{H,H}$ = 7.6 Hz, 2H). **^{13}C{^{1}H} NMR** (125 MHz, DMSO-d_6): δ = 199.1, 167.3, 141.2, 138.5, 138.1, 128.5, 128.3, 127.9, 127.9, 126.0, 40.0, 29.5.

4-(3-phenylpropanoyl)benzonitrile (12):[17]



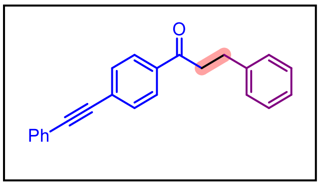
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 75% (88.2 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 8.00 (d, $J_{H,H}$ = 8.9 Hz, 2H), 7.73 (d, $J_{H,H}$ = 8.5 Hz, 2H), 7.28 (t, $J_{H,H}$ = 7.6 Hz, 2H), 7.20 (dd, $J_{H,H}$ = 14.3, 7.2 Hz, 3H), 3.29 (t, $J_{H,H}$ = 7.7 Hz, 2H), 3.06 (t, $J_{H,H}$ = 7.7 Hz, 2H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 197.9, 140.7, 139.8, 132.6, 128.7, 128.5, 126.4, 118.0, 116.4, 40.8, 29.9.

3-phenyl-1-(4-styrylphenyl)propan-1-one (13):[4]



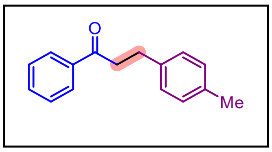
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 88% (137.5 mg) isolated yield; white solid. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 8.00 (d, $J_{H,H}$ = 8.9 Hz, 2H), 7.73 (d, $J_{H,H}$ = 8.5 Hz, 2H), 7.28 (t, $J_{H,H}$ = 7.6 Hz, 2H), 7.20 (dd, $J_{H,H}$ = 14.3, 7.2 Hz, 3H), 3.29 (t, $J_{H,H}$ = 7.9 Hz 2H), 3.06 (t, $J_{H,H}$ = 7.7 Hz, 2H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 198.7, 142.1, 141.4, 136.8, 135.7, 131.5, 128.9, 128.7, 128.6, 128.5, 128.4, 127.5, 126.9, 126.6, 126.2, 40.5, 30.3.

3-phenyl-1-(4-(phenylethynyl)phenyl)propan-1-one (14):[4]



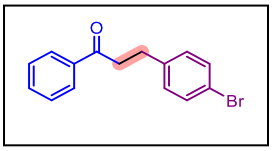
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 85% (131.9 mg) isolated yield; white solid. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 7.91 (d, $J_{H,H}$ = 7.9 Hz, 2H), 7.55 (dd, $J_{H,H}$ = 20.4, 6.6 Hz, 4H), 7.36 – 7.21 (m, 8H), 3.28 (t, $J_{H,H}$ = 7.8 Hz, 2H), 3.05 (t, $J_{H,H}$ = 7.7 Hz, 2H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 198.5, 141.3, 136.0, 131.8, 128.9, 128.8, 128.6, 128.5, 128.2, 128.1, 127.9, 126.3, 122.7, 92.8, 88.7, 40.6, 30.2.

1-phenyl-3-(p-tolyl)propan-1-one (15):[4]



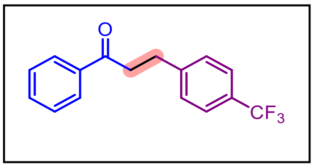
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 86% (96.4 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.94 (d, $J_{H,H}$ = 7.3 Hz, 2H), 7.54 (t, $J_{H,H}$ = 7.4 Hz, 1H), 7.44 (t, $J_{H,H}$ = 7.7 Hz, 2H), 7.15 – 7.08 (m, 4H), 3.27 (t, $J_{H,H}$ = 8.2 Hz, 2H), 3.02 (t, $J_{H,H}$ = 7.6 Hz, 2H), 2.31 (s, 3H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 199.4, 138.3, 137.0, 135.7, 133.1, 129.3, 128.7, 128.4, 128.1, 40.7, 29.8, 21.1.

3-(4-bromophenyl)-1-phenylpropan-1-one (16):[13]



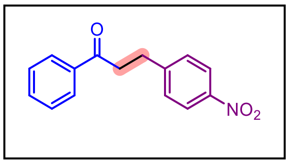
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 85% (122.9 mg) isolated yield; white solid. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 7.93 (d, $J_{H,H}$ = 7.3 Hz, 2H), 7.54 (t, $J_{H,H}$ = 7.3 Hz, 1H), 7.44 (t, $J_{H,H}$ = 7.7 Hz, 2H), 7.39 (d, $J_{H,H}$ = 8.5 Hz, 2H), 7.11 (d, $J_{H,H}$ = 8.5 Hz, 2H), 3.26 (t, $J_{H,H}$ = 7.4 Hz, 2H), 3.01 (t, $J_{H,H}$ = 7.4 Hz, 2H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 198.9, 140.3, 136.8, 133.3, 131.6, 130.3, 128.7, 128.1, 120.0, 40.2, 29.5.

1-phenyl-3-(4-(trifluoromethyl)phenyl)propan-1-one (17):[17]



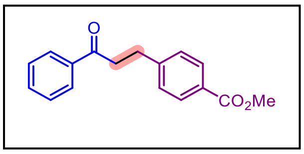
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 95% (132.2 mg) isolated yield; white solid. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 7.94 (d, $J_{H,H}$ = 7.7 Hz, 2H), 7.55 (dd, $J_{H,H}$ = 11.6, 7.8 Hz, 3H), 7.47 – 7.41 (m, 2H), 7.35 (d, $J_{H,H}$ = 8.2 Hz, 2H), 3.31 (t, $J_{H,H}$ = 7.5 Hz, 2H), 3.12 (t, $J_{H,H}$ = 7.5 Hz, 2H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 198.7, 145.5, 136.7, 133.3, 128.9, 128.8, 128.1, 125.5, 125.5, 125.5, 39.9, 29.8.

3-(4-nitrophenyl)-1-phenylpropan-1-one (18):[4]



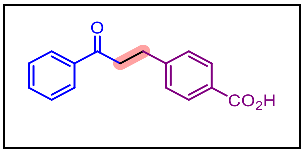
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 85% (108.4 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 8.13 (d, $J_{H,H}$ = 8.2 Hz, 2H), 7.93 (d, $J_{H,H}$ = 7.9 Hz, 2H), 7.55 (d, $J_{H,H}$ = 7.2 Hz, 1H), 7.44 (t, $J_{H,H}$ = 7.6 Hz, 2H), 7.40 (d, $J_{H,H}$ = 8.4 Hz, 2H), 3.34 (t, $J_{H,H}$ = 7.5 Hz, 2H), 3.17 (t, $J_{H,H}$ = 7.3 Hz, 2H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 198.2, 149.3, 146.6, 136.6, 133.4, 129.4, 128.8, 128.1, 123.8, 39.5, 29.8.

Methyl 4-(3-oxo-3-phenylpropyl)benzoate (19):[18]



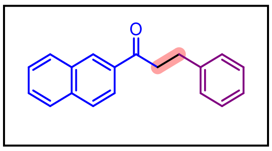
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 82% (110 mg) isolated yield; white solid. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 7.94 (d, $J_{H,H}$ = 7.7 Hz, 2H), 7.55 (dd, $J_{H,H}$ = 11.6, 7.8 Hz, 3H), 7.47 – 7.41 (m, 2H), 7.35 (d, $J_{H,H}$ = 8.2 Hz, 2H), 3.31 (t, $J_{H,H}$ = 7.5 Hz, 2H), 3.12 (t, $J_{H,H}$ = 7.5 Hz, 2H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 198.8, 167.1, 146.9, 136.8, 133.3, 129.9, 128.7, 128.6, 128.2, 128.1, 52.1, 39.9, 30.1.

4-(3-oxo-3-phenylpropyl)benzoic acid (20):[19]



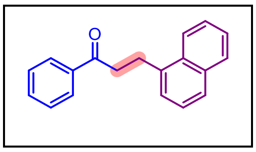
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 78% (99.2 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, DMSO-d_6): δ = 7.98 (d, $J_{H,H}$ = 7.6 Hz, 2H), 7.87 (s, 2H), 7.62 (t, $J_{H,H}$ = 7.3 Hz, 1H), 7.51 (t, $J_{H,H}$ = 7.6 Hz, 2H), 7.41 (d, $J_{H,H}$ = 8.0 Hz, 2H), 3.40 (t, $J_{H,H}$ = 7.4 Hz, 2H), 3.01 (t, $J_{H,H}$ = 7.5 Hz, 2H). ^{13}**C{^{1}H} NMR** (125 MHz, DMSO-d_6): δ = 198.9, 146.7, 136.5, 133.2, 128.7, 127.9, 39.8, 29.4.

1-(naphthalen-2-yl)-3-phenylpropan-1-one (21):[15]



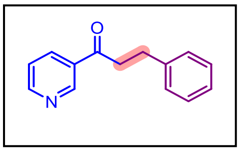
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 87% (113.2 mg) isolated yield; white solid. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 8.45 (s, 1H), 8.03 (d, $J_{H,H}$ = 8.4 Hz, 1H), 7.96 – 7.83 (m, 3H), 7.56 (dt, $J_{H,H}$ = 20.8, 7.0 Hz, 2H), 7.35 – 7.16 (m, 5H), 3.43 (t, $J_{H,H}$ = 7.9 Hz, 2H), 3.12 (t, $J_{H,H}$ = 7.5 Hz, 2H).^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 199.2, 141.4, 135.7, 134.3, 132.6, 129.8, 129.6, 129.1, 128.6, 128.6, 128.5, 127.9, 126.9, 126.3, 123.9, 40.6, 30.4.

3-(naphthalen-1-yl)-1-phenylpropan-1-one (22):[20]



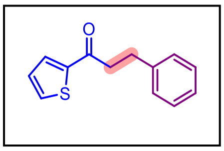
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 88% (114.5 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 8.04 (d, $J_{H,H}$ = 7.9 Hz, 1H), 7.96 – 7.93 (m, 2H), 7.86 (d, $J_{H,H}$ = 8.3 Hz, 1H), 7.75 – 7.70 (m, 1H), 7.54 – 7.38 (m, 7H), 3.53 (t, $J_{H,H}$ = 7.9 Hz, 2H), 3.42 (t, $J_{H,H}$ = 7.5 Hz, 2H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 199.4, 137.4, 136.9, 133.2, 129.0, 128.7, 128.1, 127.1, 126.2, 126.2, 125.7, 125.7, 123.6, 39.8, 27.3.

3-phenyl-1-(pyridin-3-yl)propan-1-one (23):[13]



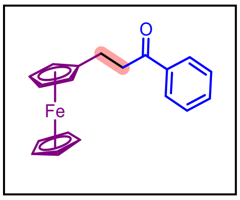
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 84% (88.7 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 9.11 (d, $J_{H,H}$ = 2.2 Hz, 1H), 8.76 – 8.68 (m, 1H), 8.17 (dd, $J_{H,H}$ = 7.9, 2.4 Hz, 1H), 7.36 (dt, $J_{H,H}$ = 7.6, 3.1 Hz, 1H), 7.22 (m, 6H), 3.27 (t, $J_{H,H}$ = 7.6 Hz, 2H), 3.04 (t, $J_{H,H}$ = 7.6 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 198.0, 153.5, 149.6, 140.7, 135.3, 132.0, 128.6, 128.4, 126.3, 123.6, 40.7, 29.8.

3-phenyl-1-(thiophen-2-yl)propan-1-one (24):[4]



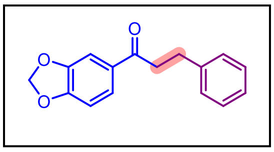
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 86% (42 mg) isolated yield; white solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.96 (d, $J_{H,H}$ = 7.7 Hz, 2H), 7.55 (t, $J_{H,H}$ = 7.6 Hz, 1H), 7.45 (t, $J_{H,H}$ = 7.6 Hz, 2H), 7.11 (d, $J_{H,H}$ = 5.1 Hz, 1H), 6.91 (t, $J_{H,H}$ = 4.3 Hz, 1H), 6.86 (d, $J_{H,H}$ = 3.4 Hz, 1H), 3.34 (t, $J_{H,H}$ = 6.9 Hz, 2H), 3.29 (t, $J_{H,H}$ = 8.1 Hz, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 198.6, 143.9, 136.8, 133.2, 128.7, 128.1, 128.1, 126.9, 124.7, 123.4, 40.6, 24.2.

3-phenyl-1-(ferrocynyl)propan-1-one (25):[21]



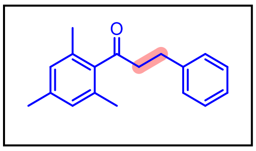
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (139.3 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.98 – 7.91 (m, 2H), 7.57 – 7.51 (m, 1H), 7.45 (t, $J_{H,H}$ = 7.7 Hz, 2H), 4.11 (s, 4H), 4.10 – 4.08 (m, 2H), 4.05 (q, $J_{H,H}$ = 2.3, 1.8 Hz, 2H), 3.18 (t, $J_{H,H}$ = 8.1 Hz, 2H), 2.77 (t, $J_{H,H}$ = 7.5 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 199.6, 137.0, 133.1, 128.7, 128.1, 88.1, 68.6, 68.2, 67.4, 40.4, 24.2.

1-(benzo[1,3]dioxol-5-yl)-3-phenylpropan-1-one (26):[4]



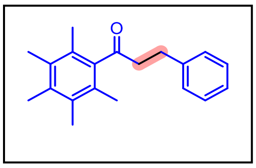
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 82% (104.3 mg) isolated yield; white solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.54 (d, $J_{H,H}$ = 7.8 Hz, 1H), 7.43 (d, $J_{H,H}$ = 1.5 Hz, 1H), 7.29 (t, $J_{H,H}$ = 7.5 Hz, 2H), 7.25 – 7.18 (m, 3H), 6.82 (d, $J_{H,H}$ = 7.7 Hz, 1H), 6.02 (s, 2H), 3.21 (t, $J_{H,H}$ = 8.3 Hz, 2H), 3.04 (t, $J_{H,H}$ = 7.5 Hz, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 197.4, 151.8, 148.3, 141.4, 131.8, 128.6, 128.5, 126.2, 124.3, 107.9, 107.9, 101.9, 40.3, 30.4.

1-mesityl-3-phenylpropan-1-one (27):[22]



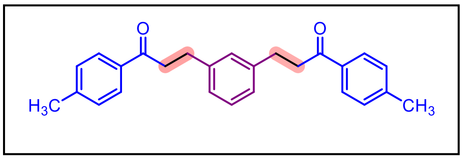
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (100.9 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.31 – 7.18 (m, 5H), 6.82 (s, 2H), 3.07 – 3.00 (m, 4H), 2.27 (s, 3H), 2.13 (s, 6H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 209.8, 141.0, 139.5, 138.4, 132.6, 128.6, 128.5, 126.2, 46.4, 29.6, 21.1, 19.1.

1-(2,3,4,5,6-pentamethylphenyl)-3-phenylpropan-1-one (28):[23]



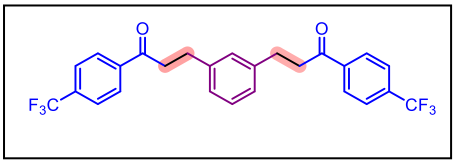
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 77% (107.9 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.21 (m, 5H), 3.07 – 3.02 (m, 2H), 3.00 – 2.95 (m, 2H), 2.20 (s, 3H), 2.15 (s, 6H), 2.02 (s, 6H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 211.0, 141.1, 140.5, 135.5, 133.2, 128.6, 128.5, 127.4, 126.1, 47.1, 29.4, 17.2, 16.7, 16.0.

3,3'-(1,3-phenylene)bis(1-(*p*-tolyl)propan-1-one) (29):



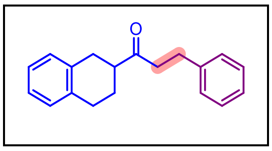
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (148.2 mg) isolated yield; white solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.88 (d, $J_{H,H}$ = 7.9 Hz, 4H), 7.29 – 7.26 (m, 5H), 7.16 – 7.11 (m, 3H), 3.28 (t, $J_{H,H}$ = 7.8 Hz, 4H), 3.06 (t, $J_{H,H}$ = 7.9 Hz, 4H), 2.43 (s, 6H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 199.0, 143.9, 141.7, 134.5, 129.3, 128.8, 128.7, 128.3, 126.3, 40.4, 30.3, 21.7. **ESI-MS:** Calcd for $C_{26}H_{27}O_2^+$, [M+H]$^+$, 371.2011; found, 371.2046.

3,3'-(1,3-phenylene)bis(1-(4-(trifluoromethyl)phenyl)propan-1-one) (30):



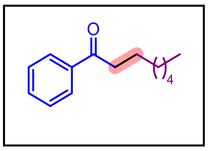
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 87% (208.1 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.94 (d, $J_{H,H}$ = 7.7 Hz, 2H), 7.54 (dd, $J_{H,H}$ = 7.4, 4.6 Hz, 4H), 7.44 (t, $J_{H,H}$ = 7.6 Hz, 3H), 7.36 (d, $J_{H,H}$ = 7.9 Hz, 3H), 3.31 (t, $J_{H,H}$ = 7.4 Hz, 4H), 3.12 (t, $J_{H,H}$ = 7.4 Hz, 4H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 198.6, 145.5, 136.7, 133.3, 128.9, 128.7, 128.1, 125.7, 125.5, 125.5, 123.0, 39.9, 29.8. **ESI-MS**: Calcd for $C_{26}H_{20}F_6O_2^+$, [M]$^+$, 478.1367; found, 478.1366.

3-phenyl-1-(1,2,3,4-tetrahydronaphthalen-2-yl)propan-1-one (31):[13]



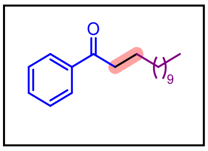
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 82% (108.4 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.08 (d, $J_{H,H}$ = 7.9 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.31 (t, $J_{H,H}$ = 7.5 Hz, 3H), 7.25 – 7.20 (m, 4H), 3.50 (dd, $J_{H,H}$ = 13.7, 3.9 Hz, 1H), 2.92 (dt, $J_{H,H}$ = 8.9, 4.4 Hz, 2H), 2.77 – 2.70 (m, 1H), 2.65 (dd, $J_{H,H}$ = 13.6, 9.5 Hz, 1H), 2.13 – 2.08 (m, 1H), 1.81 – 1.73 (m, 1H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 199.4, 144.0, 140.1, 133.3, 132.5, 129.3, 128.7, 128.4, 127.5, 126.6, 126.1, 49.4, 35.7, 28.6, 27.7.

1-phenyloctan-1-one (32):[24]



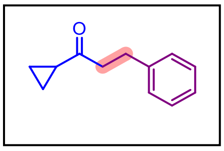
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 75% (76.6 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.94 (d, $J_{H,H}$ = 7.6 Hz, 2H), 7.53 (t, $J_{H,H}$ = 7.3 Hz, 1H), 7.43 (t, $J_{H,H}$ = 7.6 Hz, 2H), 2.94 (t, $J_{H,H}$ = 7.6 Hz, 2H), 1.71 (q, $J_{H,H}$ = 7.4 Hz, 2H), 1.34 – 1.24 (m, 8H), 0.88 – 0.84 (m, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 200.7, 137.2, 132.9, 128.6, 128.1, 38.7, 31.8, 29.4, 29.2, 24.5, 22.7, 14.1.

1-phenyltridecan-1-one (33):[25]



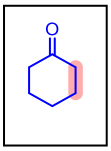
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 73% (100.2 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.95 – 7.93 (m, 2H), 7.56 – 7.50 (m, 1H), 7.44 (dd, $J_{H,H}$ = 8.4, 7.0 Hz, 2H), 2.93 (d, $J_{H,H}$ = 7.5 Hz, 2H), 1.73 – 1.69 (m, 2H), 1.24 (s, 18H), 0.85 (d, $J_{H,H}$ = 7.1 Hz, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 200.7, 137.2, 132.9, 128.6, 128.1, 38.7, 32.0, 29.7, 29.7, 29.6, 29.5, 29.4, 24.5, 22.8, 14.2.

1-cyclopropyl-3-phenylpropan-1-one (34):[14]



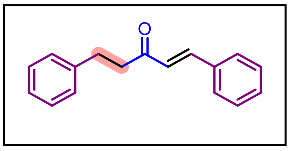
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 79% (68.8 mg) isolated yield; white solid. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 7.28 – 7.22 (m, 2H), 7.20 – 7.13 (m, 3H), 2.88 (h, $J_{H,H}$ = 4.8, 4.3 Hz, 4H), 1.89 (tt, $J_{H,H}$ = 8.0, 4.4 Hz, 1H), 0.99 (q, $J_{H,H}$ = 3.5 Hz, 2H), 0.84 (dt, $J_{H,H}$ = 7.5, 3.4 Hz, 2H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 210.0, 141.3, 128.5, 128.4, 126.1, 45.0, 30.0, 20.6, 10.8.

Cyclohexanone (35):[26]



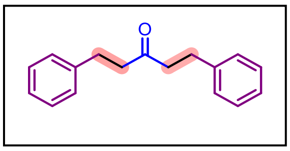
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 85% (41.7 mg) isolated yield; colourless oil. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 2.28 (t, $J_{H,H}$ = 6.6 Hz, 4H), 1.81 (m, 4H), 1.66 (t, $J_{H,H}$ = 7.4, 4.2 Hz, 2H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 212.3, 42.0, 27.0, 25.0.

1,5-diphenylpent-1-en-3-one (36):[4]



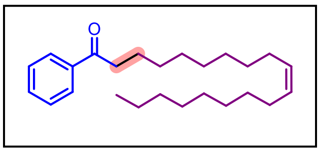
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (94.5 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.56 – 7.50 (m, 3H), 7.41 – 7.35 (m, 3H), 7.30 (t, $J_{H,H}$ = 7.4 Hz, 2H), 7.26 – 7.18 (m, 3H), 6.73 (d, $J_{H,H}$ = 16.1 Hz, 1H), 3.00 (s, 4H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 199.4, 142.8, 141.3, 130.6, 129.0, 128.6, 128.5, 128.3, 126.2, 42.5, 30.2.

1,5-diphenylpentan-3-one (37):[27]



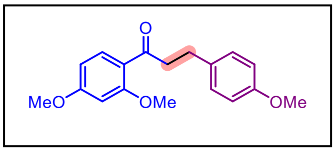
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 77% (91.8 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.28 – 7.24 (m, 5H), 7.17 (dd, $J_{H,H}$ = 21.0, 7.4 Hz, 6H), 2.88 (t, $J_{H,H}$ = 7.6 Hz, 4H), 2.70 (t, $J_{H,H}$ = 7.6 Hz, 4H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 209.3, 141.1, 128.6, 128.4, 126.2, 44.6, 29.8.

1-phenylnonadec-10-en-1-one (38):[28]



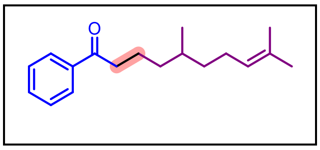
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 76% (135.5 mg) isolated yield; white solid. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 7.93 (s, 2H), 7.53 (s, 1H), 7.43 (s, 2H), 5.34 (dt, $J_{H,H}$ = 14.6, 4.3 Hz, 2H), 2.94 (s, 2H), 1.95 (m, 4H), 1.72 (q, $J_{H,H}$ = 7.3 Hz, 4H), 1.24 (s, 23H), 0.86 (s, 3H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 200.7, 137.2, 132.9, 130.5, 130.4, 128.6, 128.1, 38.7, 32.7, 32.0, 29.8, 29.7, 29.6, 29.5, 29.3, 29.2, 27.3, 24.5, 22.8, 14.2.

1-(2,4-dimethoxyphenyl)-3-(4-methoxyphenyl)propan-1-one (39):[29]



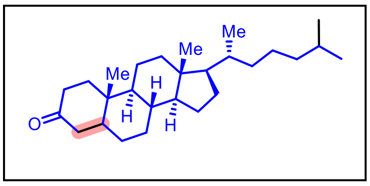
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 78% (117.1 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.79 (d, $J_{H,H}$ = 9.1 Hz, 1H), 7.13 (d, $J_{H,H}$ = 8.4 Hz, 2H), 6.81 (d, $J_{H,H}$ = 8.4 Hz, 2H), 6.51 (dd, $J_{H,H}$ = 8.8, 2.5 Hz, 1H), 6.43 (d, $J_{H,H}$ = 2.3 Hz, 1H), 3.85 (s, 3H), 3.83 (s, 3H), 3.77 (s, 3H), 3.23 – 3.20 (m, 2H), 2.93 (d, $J_{H,H}$ = 7.9 Hz, 2H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 199.7, 164.4, 160.8, 157.9, 134.1, 132.8, 129.4, 121.2, 113.9, 105.2, 98.4, 55.6, 55.5, 55.3, 45.7, 29.8.

5,9-dimethyl-1-phenyldec-8-en-1-one (40):[30]



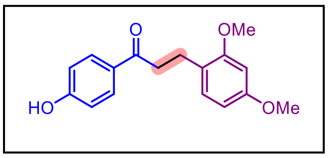
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 75% (96.9 mg) isolated yield; white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.94 (d, $J_{H,H}$ = 7.6 Hz, 2H), 7.53 (t, $J_{H,H}$ = 7.4 Hz, 1H), 7.44 (t, $J_{H,H}$ = 7.6 Hz, 2H), 5.08 (t, $J_{H,H}$ = 7.4 Hz, 1H), 2.93 (t, $J_{H,H}$ = 7.4 Hz, 2H), 1.94 (dt, $J_{H,H}$ = 14.7, 6.8 Hz, 2H), 1.76 – 1.68 (m, 2H), 1.66 (s, 3H), 1.58 (s, 3H), 1.44 – 1.32 (m, 3H), 1.18 (m, 2H), 0.88 (d, $J_{H,H}$ = 6.2 Hz, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 200.7, 137.2, 132.9, 131.2, 128.6, 128.1, 125.0, 39.0, 37.0, 36.7, 32.4, 25.8, 25.6, 21.9, 19.5, 17.7.

Cholestan-3-one (41):[31]



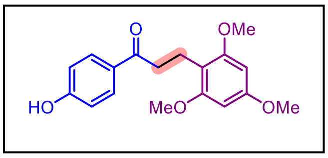
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 72% (139.2 mg) isolated yield; white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 2.73 (dt, $J_{H,H}$ = 14.8, 3.5 Hz, 1H), 2.48 – 2.28 (m, 2H), 2.12 – 1.92 (m, 3H), 1.87 – 1.79 (m, 2H), 1.76 (s, 3H), 1.68 – 1.46 (m, 7H), 1.44 – 1.21 (m, 7H), 1.15 (s, 4H), 1.11 – 1.03 (m, 4H), 1.01 – 0.92 (m, 3H), 0.89 (d, $J_{H,H}$ = 6.3 Hz, 3H), 0.86 – 0.84 (m, 5H), 0.70 (s, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 215.0, 56.4, 56.3, 54.7, 54.2, 49.4, 44.8, 42.7, 40.8, 40.0, 39.6, 36.9, 36.2, 35.9, 34.9, 28.4, 28.4, 28.1, 24.3, 23.9, 22.9, 22.6, 21.5, 18.8, 15.0, 13.7, 12.2, 11.6.

Loureirin A (42):[32]



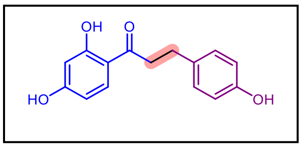
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 76% (108.8 mg) isolated yield; white solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.90 (d, $J_{H,H}$ = 8.5 Hz, 2H), 7.06 (d, $J_{H,H}$ = 8.2 Hz, 1H), 6.88 (d, $J_{H,H}$ = 8.5 Hz, 2H), 6.44 – 6.38 (m, 2H), 3.78 (s, 6H), 3.17 (t, $J_{H,H}$ = 7.7 Hz, 2H), 2.97 – 2.93 (m, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 200.0, 160.8, 159.5, 158.4, 130.9, 130.4, 121.9, 115.5, 103.9, 98.6, 55.5, 55.3, 39.0, 25.6.

Loureirin B (43):[33]



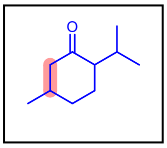
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 70% (110.72 mg) isolated yield; white solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.89 (d, $J_{H,H}$ = 8.6 Hz, 2H), 6.87 (d, $J_{H,H}$ = 8.8 Hz, 2H), 6.74 (s, 1H), 6.50 (s, 1H), 3.85 (s, 3H), 3.79 (s, 3H), 3.79 (s, 3H), 3.18 – 3.15 (m, 2H), 2.97 – 2.94 (m, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 199.6, 160.8, 151.7, 148.1, 142.8, 130.9, 129.8, 121.2, 115.4, 114.6, 97.9, 56.8, 56.3, 39.1, 25.7.

Davidigenin (44):[34]



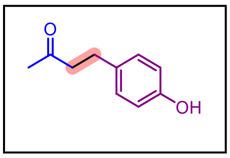
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 61% (78.8 mg) isolated yield; white solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 12.65 (s, 1H), 7.77 (d, $J_{H,H}$ = 9.0 Hz, 1H), 7.06 – 7.03 (m, 2H), 6.67 (d, $J_{H,H}$ = 8.4 Hz, 2H), 6.36 (dd, $J_{H,H}$ = 8.8, 2.6 Hz, 1H), 6.26 (d, $J_{H,H}$ = 2.3 Hz, 1H), 3.19 (t, $J_{H,H}$ = 7.6 Hz, 2H), 2.81 (t, $J_{H,H}$ = 7.6 Hz, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 203.9, 164.8, 164.4, 155.6, 133.0, 131.1, 129.3, 115.1, 112.6, 108.2, 102.5, 39.4, 29.1.

Menthone (45):[35]



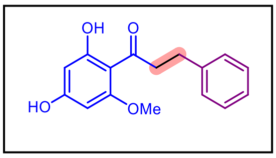
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 81% (62.5 mg) isolated yield; white solid. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 2.34 – 2.27 (m, 1H), 2.15 – 1.80 (m, 6H), 1.38 – 1.25 (m, 2H), 0.97 (d, $J_{H,H}$ = 6.7 Hz, 3H), 0.87 (d, $J_{H,H}$ = 6.5 Hz, 3H), 0.81 (d, $J_{H,H}$ = 6.6 Hz, 3H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 212.5, 55.9, 50.9, 35.5, 34.0, 27.9, 25.9, 22.3, 21.3, 18.7.

Rheosmin (46):[36]



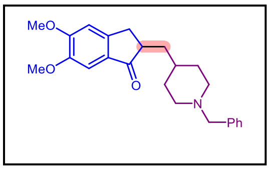
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 76% (59.9 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.03 (d, $J_{H,H}$ = 8.3 Hz, 2H), 6.74 (d, $J_{H,H}$ = 8.3 Hz, 2H), 2.82 (t, $J_{H,H}$ = 7.5 Hz, 2H), 2.72 (t, $J_{H,H}$ = 7.5 Hz, 2H), 2.13 (s, 3H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 209.3, 154.2, 132.9, 132.6, 129.5, 116.1, 115.5, 45.6, 30.3, 29.1.

Uvangoletin (47):[37]



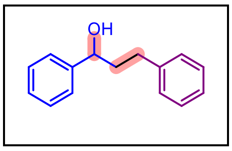
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 65% (88.5 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.03 (d, $J_{H,H}$ = 8.3 Hz, 2H), 6.74 (d, $J_{H,H}$ = 8.3 Hz, 2H), 2.82 (t, $J_{H,H}$ = 7.5 Hz, 2H), 2.72 (t, $J_{H,H}$ = 7.5 Hz, 2H), 2.13 (s, 3H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 206.5, 164.8, 161.4, 141.6, 136.0, 128.5, 126.1, 111.2, 111.0, 101.3, 55.8, 46.6, 30.5.

Donepezil (48):[38]



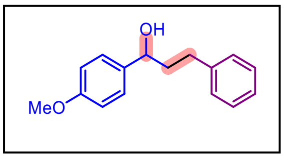
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 88% (167 mg) isolated yield; white solid. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.29 (d, $J_{H,H}$ = 4.5 Hz, 4H), 7.23 (d, $J_{H,H}$ = 9.2 Hz, 1H), 7.14 (s, 1H), 6.83 (s, 1H), 3.93 (s, 3H), 3.88 (s, 3H), 3.50 (s, 2H), 3.23 – 3.19 (m, 1H), 2.91 – 2.88 (m, 2H), 2.67 (dd, $J_{H,H}$ = 14.3, 3.7 Hz, 2H), 1.99 – 1.89 (m, 3H), 1.71 – 1.64 (m, 2H), 1.51 – 1.45 (m, 1H), 1.36 – 1.29 (m, 3H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 207.8, 155.5, 149.5, 148.8, 138.2, 129.4, 129.3, 128.2, 127.1, 107.4, 104.5, 63.4, 45.5, 38.7, 34.4, 33.4, 32.9, 31.8, 31.3.

1,3-diphenylpropan-1-ol (2a):[39]



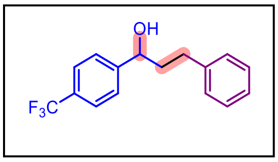
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 85% (90.2 mg) isolated yield; colourless oil. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 7.35 (d, $J_{H,H}$ = 3.8 Hz, 4H), 7.31- 7.25 (m, 3H), 7.23- 7.16 (m, 3H), 4.68 (dd, $J_{H,H}$ = 7.9, 5.5 Hz, 1H), 2.77- 2.64 (m, 2H), 2.18-2.00 (m, 3H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 144.6, 141.8, 128.6, 128.5, 128.4, 127.7, 126.0, 125.9, 73.9, 40.5, 32.1.

1-(4-methoxyphenyl)-3-phenylpropan-1-ol (49):[39]



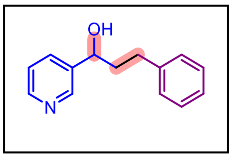
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (96.9 mg) isolated yield; colourless oil. ^{1}**H NMR** (400 MHz, $CDCl_3$): δ = 7.27 (dd, $J_{H,H}$ = 8.2, 6.4 Hz, 4H), 7.20 – 7.12 (m, 3H), 6.88 (d, $J_{H,H}$ = 8.6 Hz, 2H), 4.62 (dd, $J_{H,H}$ = 7.7, 5.7 Hz, 1H), 3.80 (s, 3H), 2.75 – 2.61 (m, 2H), 2.18 – 1.90 (m, 3H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 159.1, 141.9, 136.8, 128.5, 128.4, 127.3, 125.9, 113.9, 73.5, 55.3, 40.4, 32.1.

3-phenyl-1-(4-(trifluoromethyl)phenyl)propan-1-ol (50):[40]



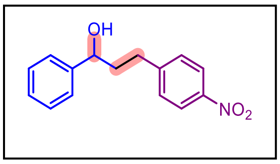
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 87% (121.9 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.60 (d, $J_{H,H}$ = 8.1 Hz, 2H), 7.44 (d, $J_{H,H}$ = 7.8 Hz, 2H), 7.29 (t, $J_{H,H}$ = 7.5 Hz, 2H), 7.20 (t, $J_{H,H}$ = 9.1 Hz, 3H), 4.73 (dd, $J_{H,H}$ = 8.0, 5.0 Hz, 1H), 2.77 – 2.66 (m, 2H), 2.15 – 2.00 (m, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 148.6, 141.4, 130.0, 129.7, 128.6, 128.5, 126.2, 126.1, 125.5, 73.2, 40.6, 31.9.

3-phenyl-1-(pyridin-3-yl)propan-1-ol (51):[41]



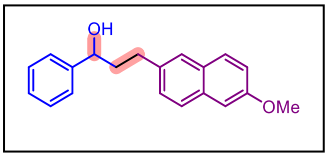
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 81% (81.1 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.36 – 8.31 (m, 2H), 7.67 (d, $J_{H,H}$ = 7.6 Hz, 1H), 7.24 – 7.12 (m, 7H), 4.66 (d, $J_{H,H}$ = 5.3 Hz, 1H), 2.69 (m, 2H), 2.15 – 1.90 (m, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 148.3, 147.5, 141.5, 140.7, 134.0, 128.5, 128.4, 126.0, 123.6, 70.9, 40.5, 31.9.

3-(4-nitrophenyl)-1-phenylpropan-1-ol (52):[42]



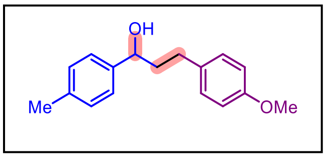
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 85% (103.8 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 8.12 (d, $J_{H,H}$ = 8.5 Hz, 2H), 7.37 – 7.28 (m, 7H), 2.86 (m, 1H), 2.77 (m, 1H), 2.17 – 2.09 (m, 1H), 2.06 – 1.98 (m, 1H), 1.88 (s, 1H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 129.3, 128.8, 128.0, 125.9, 123.8, 73.7, 39.9, 32.1.

3-(6-methoxynaphthalen-2-yl)-1-phenylpropan-1-ol (53):



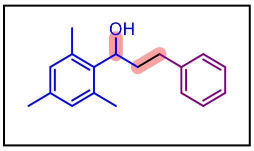
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (101.3 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.65 (dd, $J_{H,H}$ = 8.4, 2.4 Hz, 2H), 7.55 (s, 1H), 7.35 (d, $J_{H,H}$ = 4.2 Hz, 4H), 7.31 – 7.25 (m, 2H), 7.14 – 7.09 (m, 2H), 4.70 (t, $J_{H,H}$ = 6.7 Hz, 1H), 3.90 (s, 3H), 2.90 – 2.77 (m, 2H), 2.24 – 2.17 (m, 1H), 2.14 – 2.05 (m, 1H), 1.93 (d, $J_{H,H}$ = 3.1 Hz, 1H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 157.2, 144.7, 137.0, 133.1, 129.2, 129.0, 128.6, 127.9, 127.7, 126.9, 126.4, 126.0, 118.8, 105.7, 55.4, 40.5, 32.0. **ESI-MS:** Calcd for $C_{20}H_{21}O_2^+$, $[M+H]^+$, 293.1542; found, 293.1548.

3-(4-methoxyphenyl)-1-(p-tolyl)propan-1-ol (54):[43]



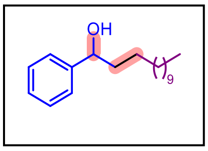
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 79% (101.3 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.23 (d, $J_{H,H}$ = 7.7 Hz, 2H), 7.16 (d, $J_{H,H}$ = 7.8 Hz, 2H), 7.11 (d, $J_{H,H}$ = 8.6 Hz, 2H), 6.83 (d, $J_{H,H}$ = 9.0 Hz, 2H), 4.62 (dd, $J_{H,H}$ = 7.7, 5.4 Hz, 1H), 3.78 (s, 3H), 2.71 – 2.58 (m, 2H), 2.36 (s, 3H), 2.12 – 1.95 (m, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 157.8, 137.2, 133.9, 129.3, 129.2, 125.9, 113.8, 73.7, 31.2, 21.1.

1-mesityl-3-phenylpropan-1-ol (55):[44]



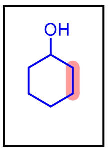
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 77% (97.9 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.31 – 7.25 (m, 2H), 7.23 – 7.15 (m, 3H), 6.80 (s, 2H), 5.11 (dd, $J_{H,H}$ = 9.3, 4.7 Hz, 1H), 2.88 (m, 1H), 2.67 (m, 1H), 2.39 – 2.34 (m, 1H), 2.32 (s, 6H), 2.23 (s, 3H), 1.96 (m, 1H), 1.71 (s, 1H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 141.9, 136.9, 136.1, 130.2, 128.6, 128.4, 125.9, 70.7, 37.1, 32.8, 20.8, 20.7.

1-phenyltridecan-1-ol (56):[45]



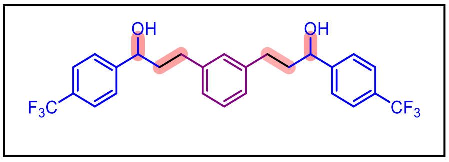
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 75% (61.6 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.33 (d, $J_{H,H}$ = 4.6 Hz, 4H), 7.30 – 7.24 (m, 1H), 4.68 – 4.62 (m, 1H), 1.74 (m, 2H), 1.40 (dd, $J_{H,H}$ = 13.0, 6.8 Hz, 1H), 1.24 (s, 20H), 0.87 (t, $J_{H,H}$ = 6.8 Hz, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 145.0, 128.5, 127.6, 126.0, 74.8, 39.2, 32.0, 29.7, 29.6, 29.4, 25.9, 22.8, 14.2.

Cyclohexanol (57):[46]



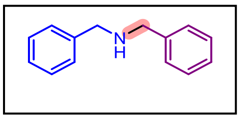
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 86% (43.1 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 3.55 (hept, $J_{H,H}$ = 4.1 Hz, 1H), 1.85 (td, $J_{H,H}$ = 11.4, 10.9, 6.2 Hz, 3H), 1.69 (dd, $J_{H,H}$ = 8.9, 4.5 Hz, 2H), 1.53 – 1.47 (m, 1H), 1.25 – 1.11 (m, 5H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 70.3, 35.5, 25.5, 24.2.

3,3'-(1,3-phenylene)bis(1-(4-(trifluoromethyl)phenyl)propan-1-ol) (58):



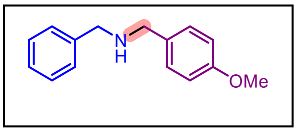
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 86% (184.3 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 3.55 (m, 1H), 1.85 (td, $J_{H,H}$ = 11.4, 10.9, 6.2 Hz, 3H), 1.69 (dd, $J_{H,H}$ = 8.9, 4.5 Hz, 2H), 1.53 – 1.47 (m, 1H), 1.25 – 1.11 (m, 5H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 146.0, 144.4, 128.8, 128.7, 127.9, 125.9, 125.4, 73.8, 40.1, 31.9. **ESI-MS:** Calcd for $C_{26}H_{25}F_6O_2^+$, [M+H]$^+$, 483.1759; found, 483.1759.

Dibenzylamine (59):[47]



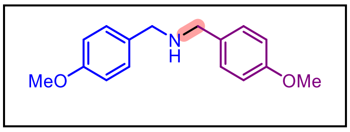
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 90% (88.8 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.36 – 7.30 (m, 8H), 7.27 – 7.23 (m, 2H), 3.81 (s, 4H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 140.4, 128.5, 128.2, 127.0, 53.2.

N-benzyl-1-(4-methoxyphenyl)methanamine (60):[48]



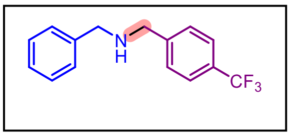
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 82% (87.9 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, D_2O): δ = 7.38 (t, $J_{H,H}$ = 3.4 Hz, 3H), 7.34 (d, $J_{H,H}$ = 2.4 Hz, 2H), 7.29 (d, $J_{H,H}$ = 8.9 Hz, 2H), 6.94 (d, $J_{H,H}$ = 8.8 Hz, 2H), 4.11 (s, 2H), 4.08 (s, 2H), 3.73 (s, 3H). **^{13}C{^{1}H} NMR** (125 MHz, D_2O): δ = 159.8, 131.6, 130.8, 129.9, 129.7, 129.3, 123.1, 114.7, 55.5, 50.3, 50.0.

bis(4-methoxybenzyl)amine (61):[49]



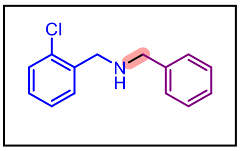
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 76% (87.5 mg) isolated yield; colourless oil. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.25 (d, $J_{H,H}$ = 8.3 Hz, 4H), 6.87 (d, $J_{H,H}$ = 8.3 Hz, 4H), 3.78 (s, 6H), 3.72 (s, 4H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 158.6, 132.4, 129.3, 129.3, 113.7, 113.7, 55.2, 55.1, 52.4.

N-benzyl-1-(4-(trifluoromethyl)phenyl)methanamine (62):[50]



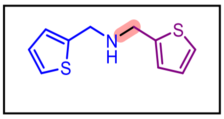
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 91% (120.7 mg) isolated yield; colourless oil. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.59 (d, $J_{H,H}$ = 7.9 Hz, 2H), 7.47 (d, $J_{H,H}$ = 8.1 Hz, 2H), 7.34 (d, $J_{H,H}$ = 4.4 Hz, 4H), 7.30 – 7.24 (m, 1H), 3.86 (s, 2H), 3.81 (s, 2H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 144.6, 140.1, 128.6, 128.4, 128.3, 127.2, 127.2, 125.5, 125.4, 53.3, 52.7.

N-benzyl-1-(2-chlorophenyl)methanamine (63): [51]



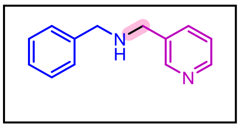
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 83% (96.2 mg) isolated yield; colourless oil. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.43 – 7.34 (m, 6H), 7.30 – 7.18 (m, 3H), 3.92 (s, 2H), 3.82 (s, 2H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 140.1, 137.6, 133.8, 130.2, 129.5, 128.4, 128.3, 128.2, 127.0, 127.0, 126.8, 53.2, 53.1, 50.8.

bis(thiophen-2-ylmethyl)amine (64):[52]



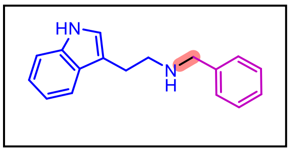
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 87% (91 mg) isolated yield; colourless oil. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 7.22 (d, $J_{H,H}$ = 5.3 Hz, 2H), 6.95 (d, $J_{H,H}$ = 5.1 Hz, 2H), 6.93 (d, $J_{H,H}$ = 3.3 Hz, 2H), 4.02 (s, 4H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 143.7, 126.7, 125.2, 124.6, 47.1.

N-benzyl-1-(pyridin-3-yl)methanamine (65):[53]



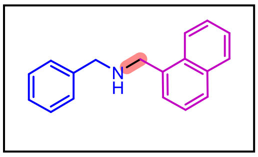
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 80% (79.3 mg) isolated yield; colourless oil. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 8.52 (d, $J_{H,H}$ = 2.2 Hz, 1H), 8.45 (dd, $J_{H,H}$ = 5.2, 1.6 Hz, 1H), 7.67 – 7.64 (m, 1H), 7.29 (s, 5H), 7.23 – 7.19 (m, 2H), 3.75 (s, 4H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 149.6, 148.3, 139.8, 135.8, 128.4, 128.0, 127.0, 123.3, 53.1, 50.3.

N-benzyl-2-(1H-indol-3-yl)ethan-1-amine (66):[54]



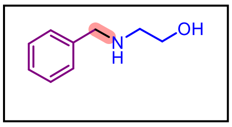
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 74% (92.6 mg) isolated yield; colourless oil. ^{1}**H NMR** (500 MHz, $CDCl_3$): δ = 8.31 (s, 1H), 7.63 (d, $J_{H,H}$ = 7.8 Hz, 1H), 7.34 – 7.28 (m, 5H), 7.27 – 7.24 (m, 1H), 7.21 (t, $J_{H,H}$ = 7.6 Hz, 1H), 7.13 (t, $J_{H,H}$ = 7.5 Hz, 1H), 6.97 (d, $J_{H,H}$ = 2.8 Hz, 1H), 3.84 (s, 2H), 3.03 (s, 4H). ^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 140.3, 136.6, 128.8, 128.6, 128.5, 128.3, 127.1, 122.2, 122.1, 119.3, 119.0, 113.8, 111.3, 54.0, 49.5, 25.9.

N-benzyl-1-(naphthalen-1-yl)methanamine (67):[55]



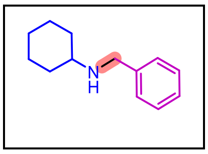
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 83% (102.6 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 8.21 (d, $J_{H,H}$ = 8.2 Hz, 1H), 7.96 (d, $J_{H,H}$ = 7.9 Hz, 1H), 7.88 (d, $J_{H,H}$ = 8.2 Hz, 1H), 7.64 – 7.56 (m, 3H), 7.50 (m, 5H), 7.39 (t, $J_{H,H}$ = 7.3 Hz, 1H), 4.33 (s, 2H), 4.00 (s, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 140.3, 135.9, 133.9, 131.8, 128.6, 128.4, 128.2, 127.7, 127.0, 126.0, 126.0, 125.6, 125.3, 123.8, 53.7, 50.8.

2-(benzylamino)ethan-1-ol (68):[56]



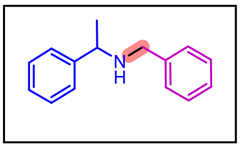
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 71% (53.7 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 8.21 (d, $J_{H,H}$ = 8.2 Hz, 1H), 7.96 (d, $J_{H,H}$ = 7.9 Hz, 1H), 7.88 (d, $J_{H,H}$ = 8.2 Hz, 1H), 7.64 – 7.56 (m, 3H), 7.50 (m, 5H), 7.39 (t, $J_{H,H}$ = 7.3 Hz, 1H), 4.33 (s, 2H), 4.00 (s, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 139.7, 128.5, 128.2, 127.1, 60.7, 53.5, 50.7.

N-benzylcyclohexanamine (69):[50]



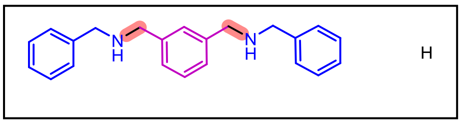
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 78% (73.8 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.33 – 7.21 (m, 5H), 3.80 (s, 2H), 2.49 (td, $J_{H,H}$ = 10.1, 5.0 Hz, 1H), 1.91 (d, $J_{H,H}$ = 12.0 Hz, 2H), 1.76 – 1.70 (m, 2H), 1.60 (d, $J_{H,H}$ = 11.4 Hz, 2H), 1.24 (d, $J_{H,H}$ = 10.7 Hz, 2H), 1.13 (t, $J_{H,H}$ = 11.0 Hz, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 128.5, 128.2, 126.9, 56.3, 51.1, 33.6, 26.3, 25.1.

N-benzyl-1-phenylethan-1-amine (70):[50]



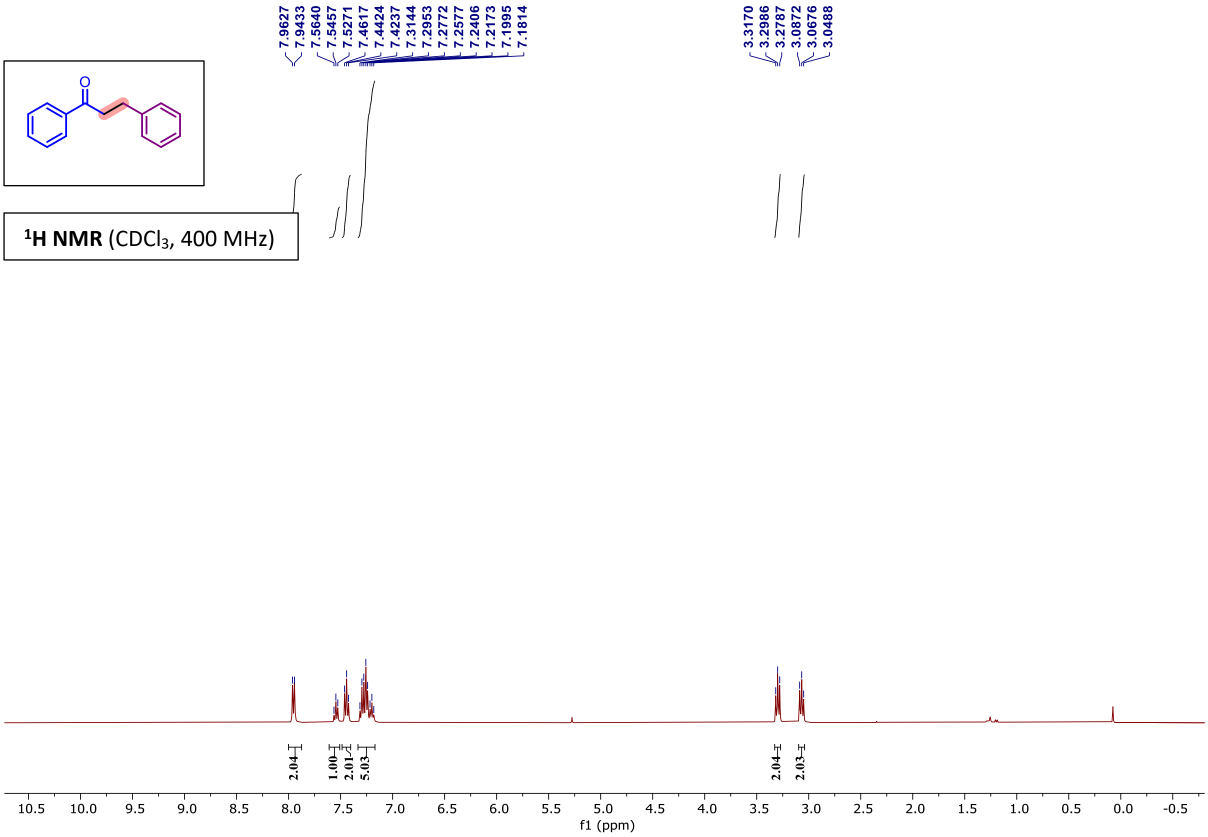
Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 80% (84.5 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.36 – 7.21 (m, 10H), 3.81 (q, $J_{H,H}$ = 6.5 Hz, 1H), 3.67 – 3.57 (m, 2H), 1.36 (d, $J_{H,H}$ = 6.8 Hz, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 145.6, 140.6, 128.5, 128.4, 128.2, 127.0, 126.9, 126.7, 57.5, 51.7, 24.5.

1,1'-(1,3-phenylene)bis(N-benzylmethanamine) (71):

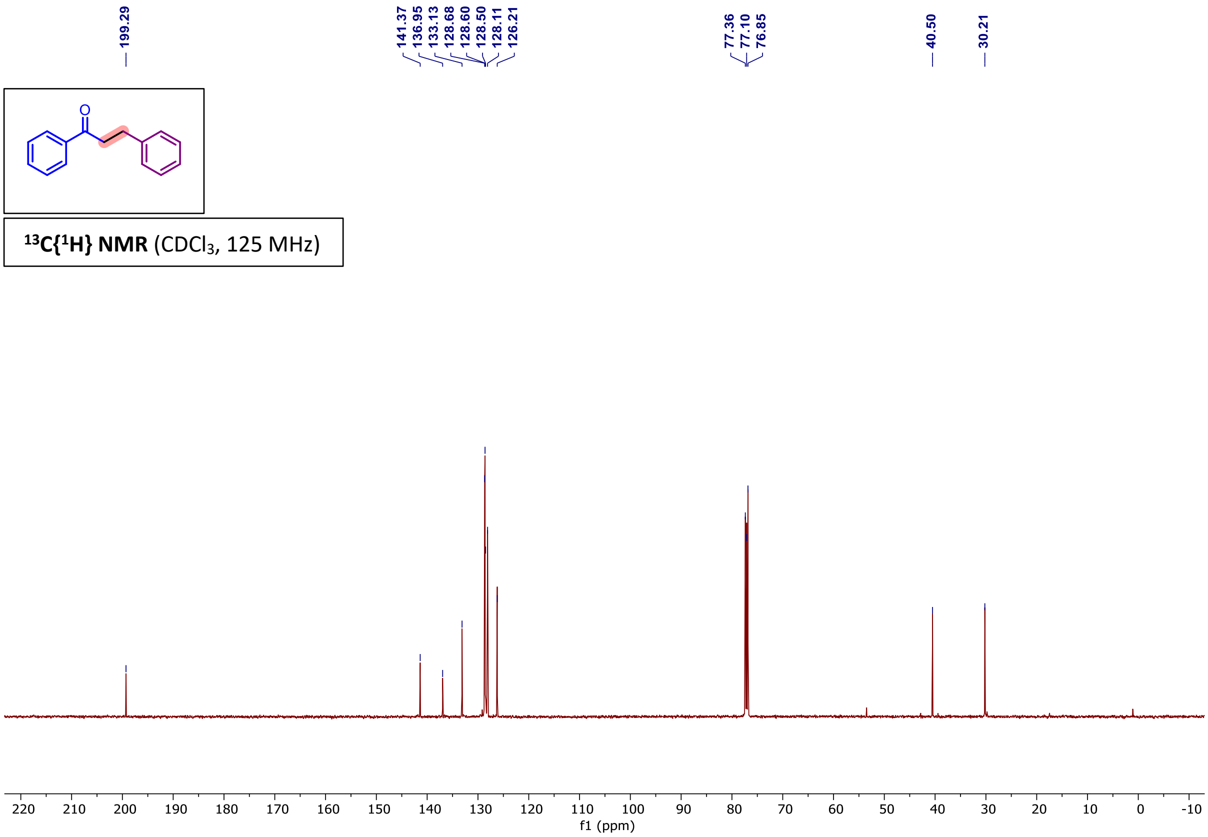


Purified by column chromatography using alumina and ethyl acetate-hexane as eluent 88% (139.2 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.36 – 7.21 (m, 10H), 3.81 (q, $J_{H,H}$ = 6.5 Hz, 1H), 3.67 – 3.57 (m, 2H), 1.36 (d, $J_{H,H}$ = 6.8 Hz, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 140.5, 140.4, 128.5, 128.5, 128.2, 128.0, 127.0, 126.9, 53.3, 53.2. **ESI-MS:** Calcd for $C_{22}H_{25}N_2^+$, $[M+H]^+$, 317.2018; found, 317.2016.

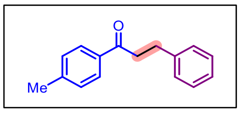
10. Copies of ^{1}H and ^{13}C{^{1}H} NMR Spectra of Products



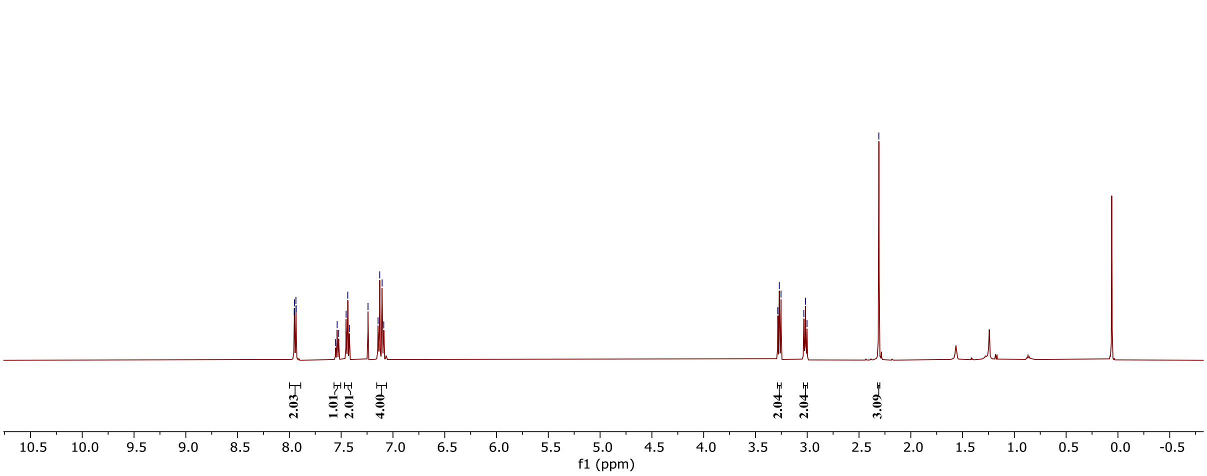
^{1}H NMR ($CDCl_3$, 400 MHz)

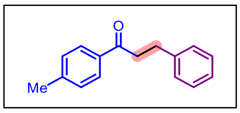


^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)

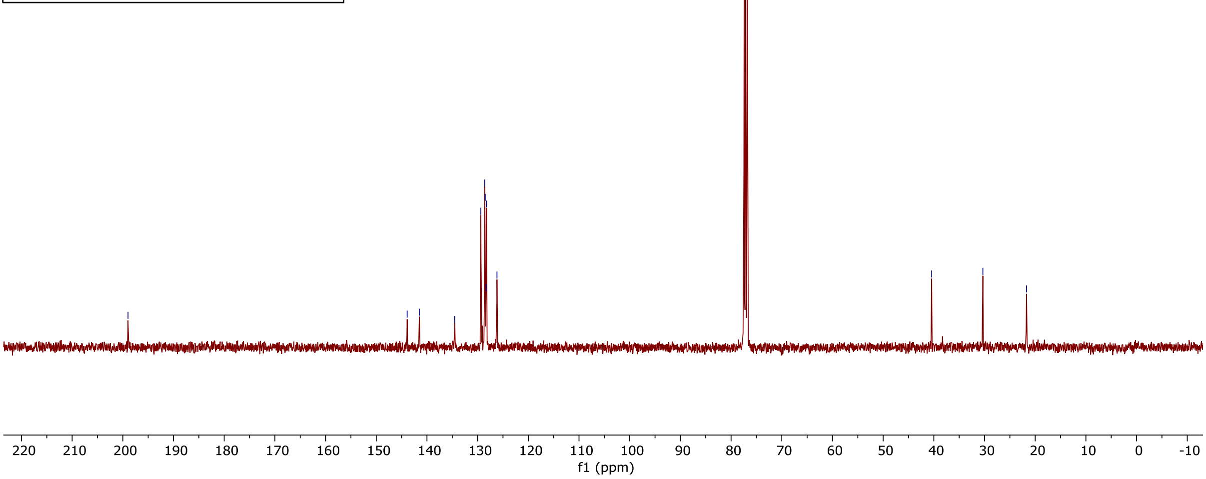


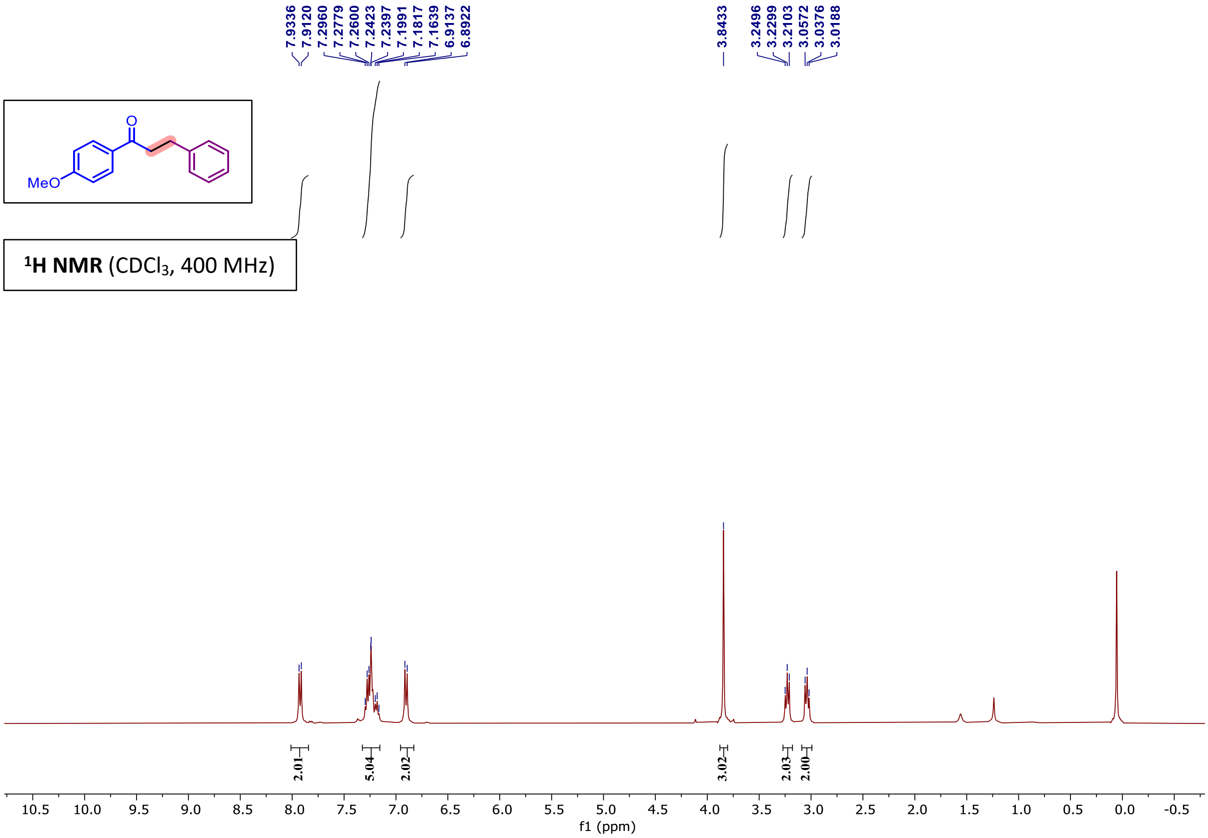
^{1}H NMR ($CDCl_3$, 500 MHz)



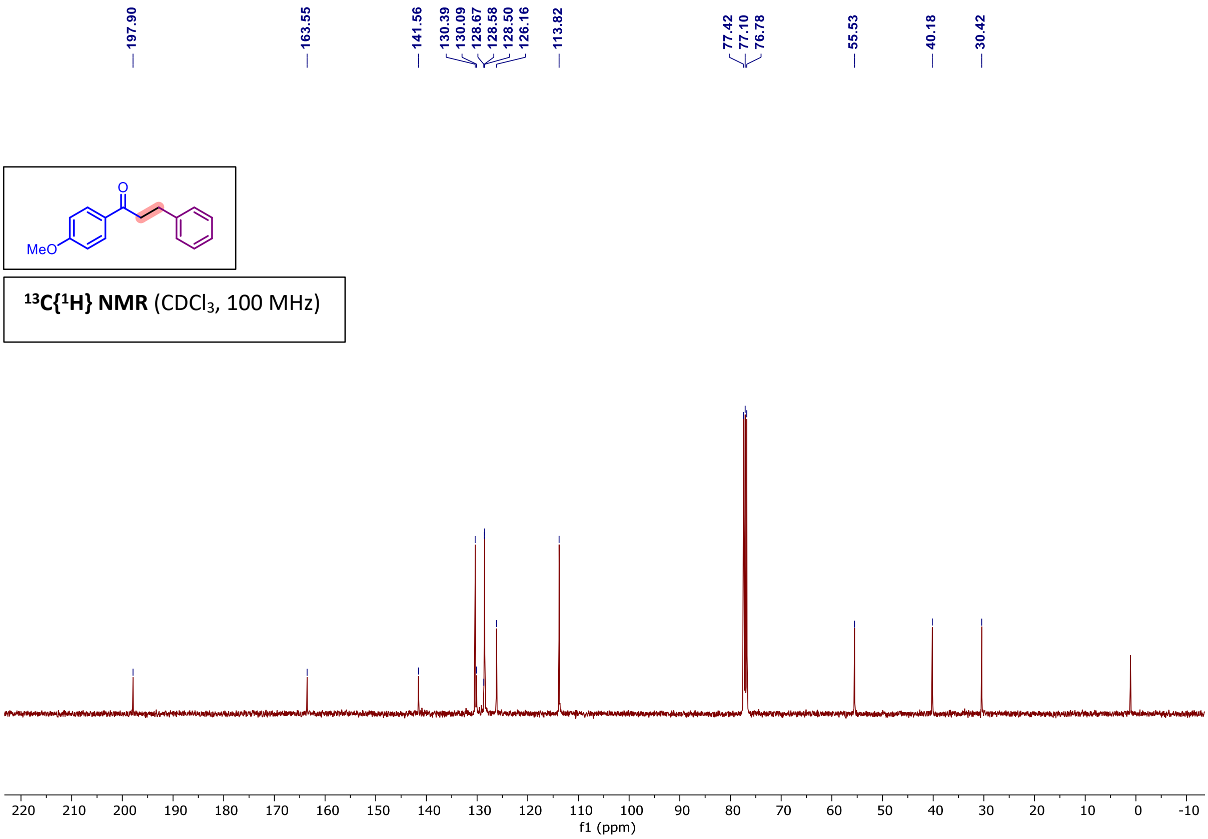


$^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz)

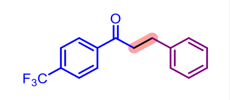




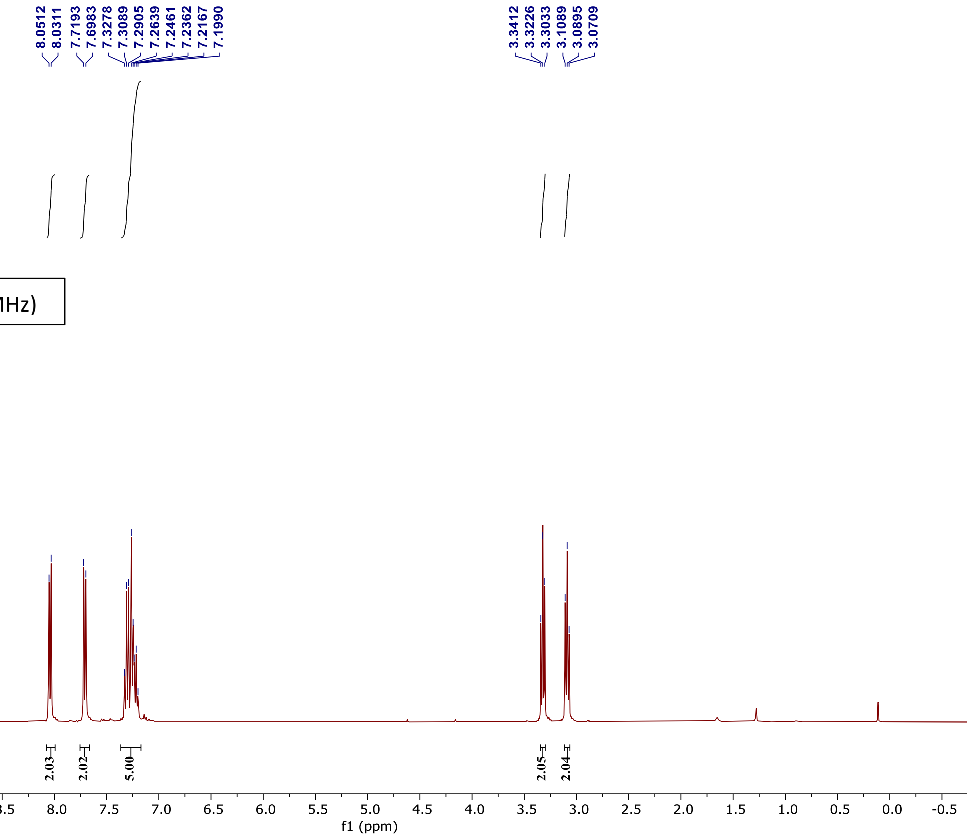
[1]H NMR ($CDCl_3$, 400 MHz)

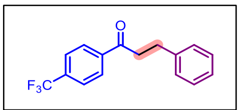


[13]C{[1]H} NMR ($CDCl_3$, 100 MHz)

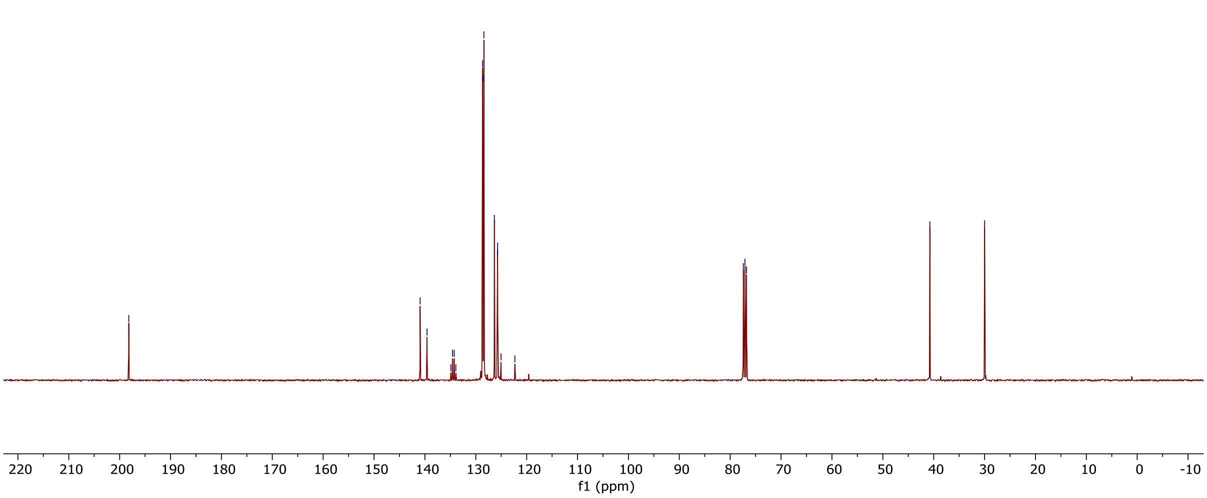


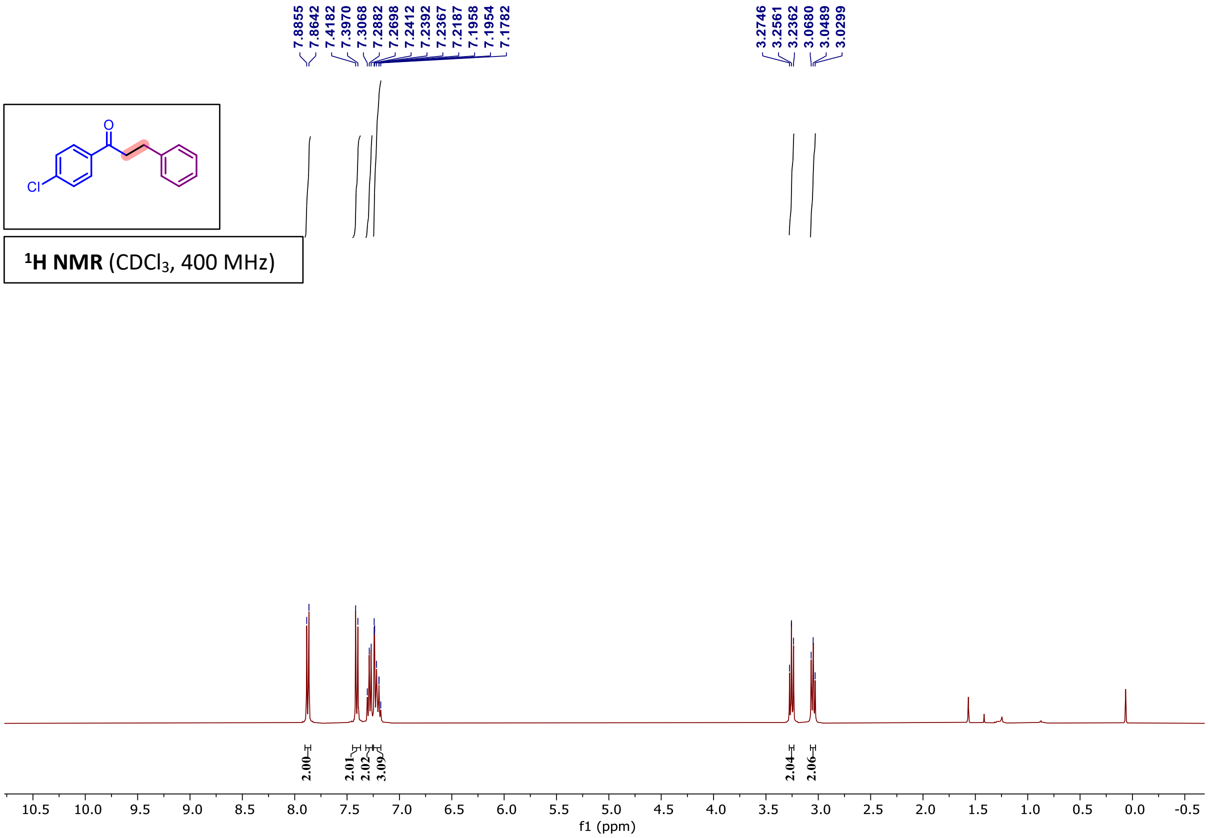
¹H NMR ($CDCl_3$, 400 MHz)



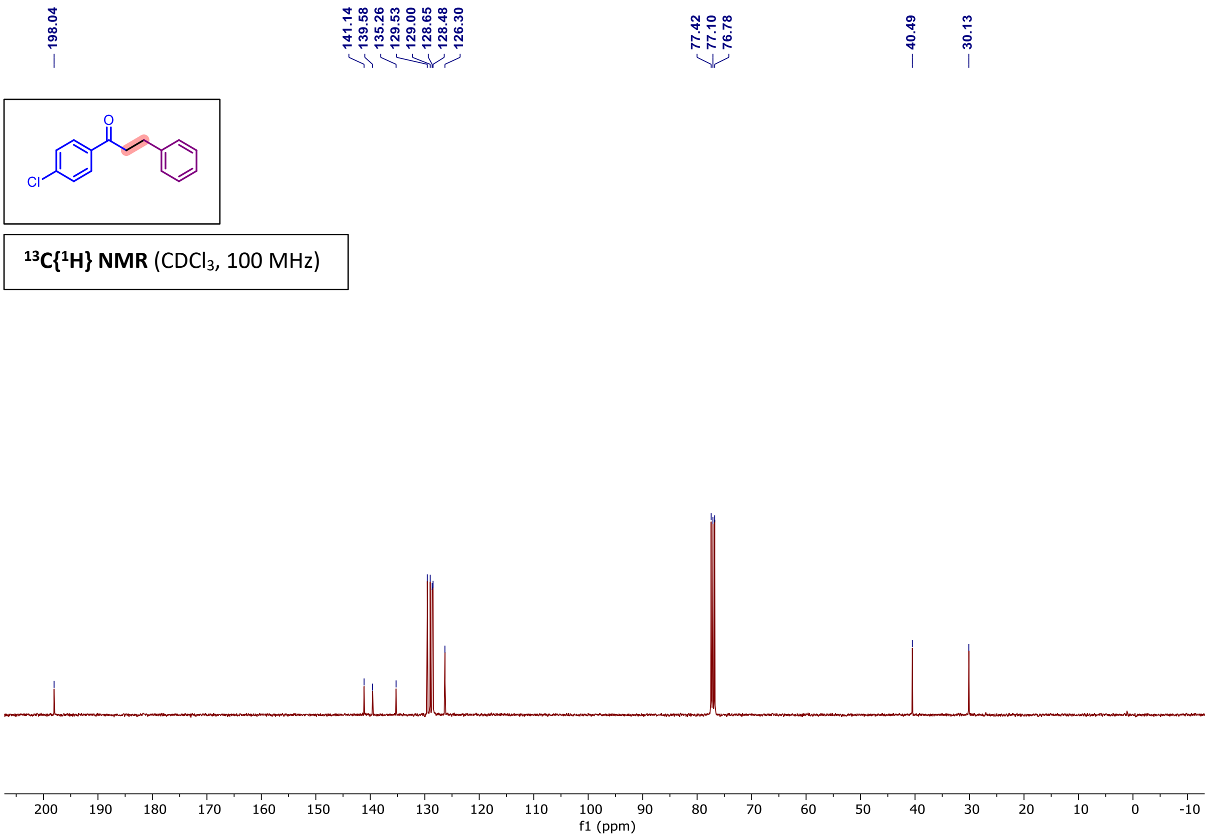


¹³C{¹H} NMR ($CDCl_3$, 100 MHz)

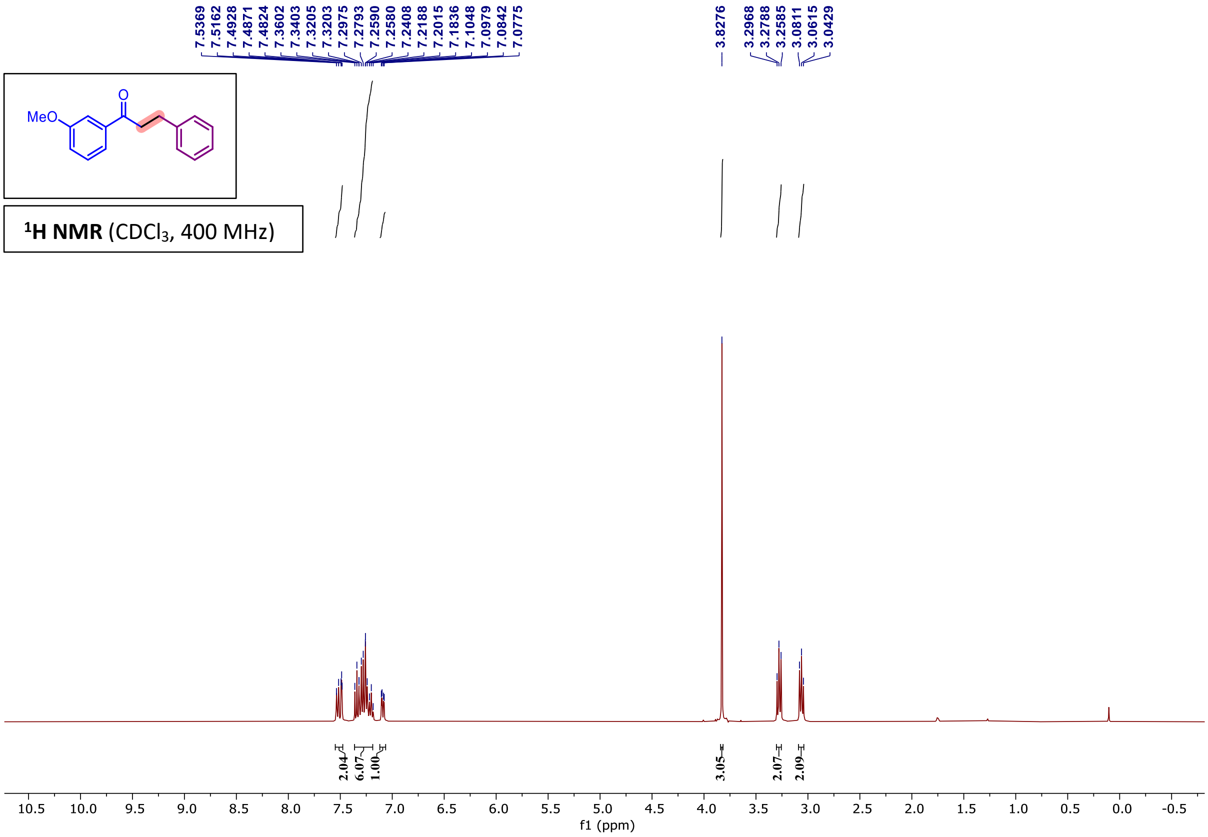


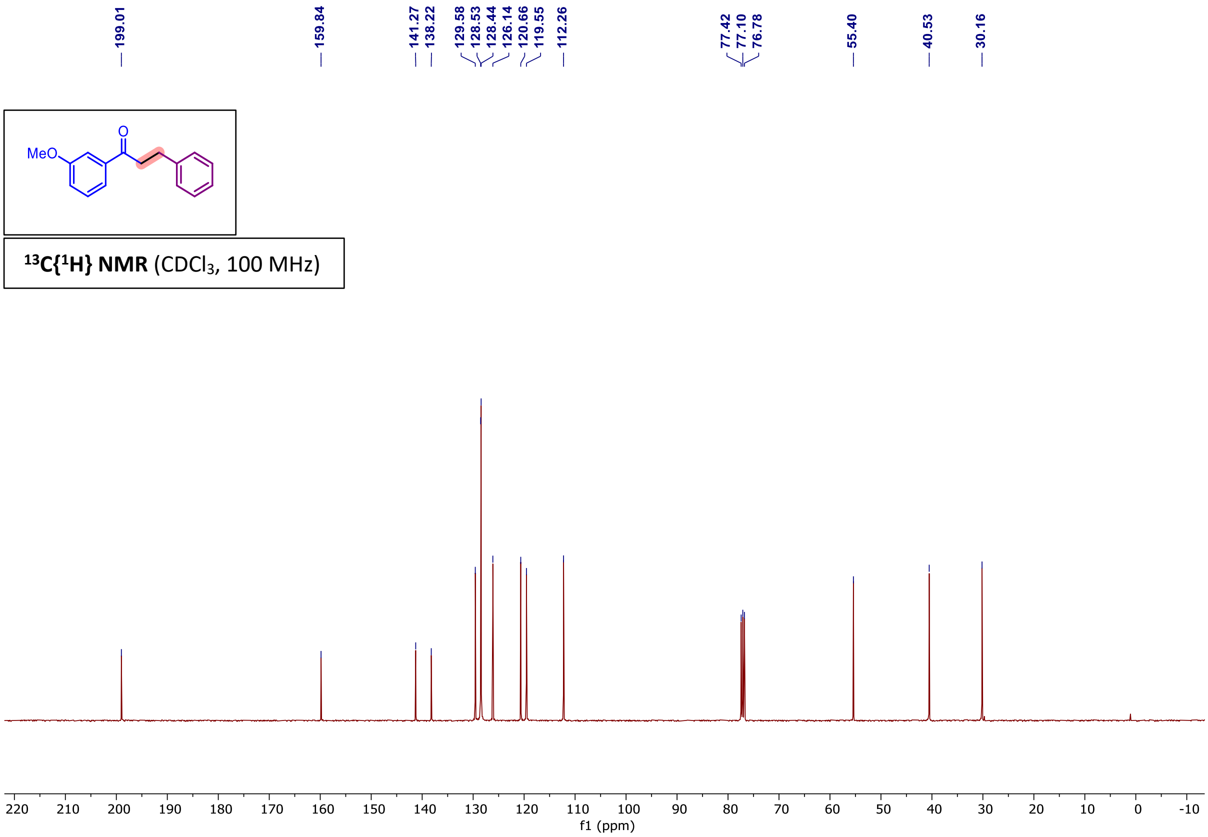


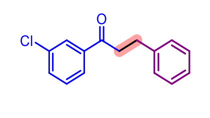
^{1}H NMR ($CDCl_3$, 400 MHz)



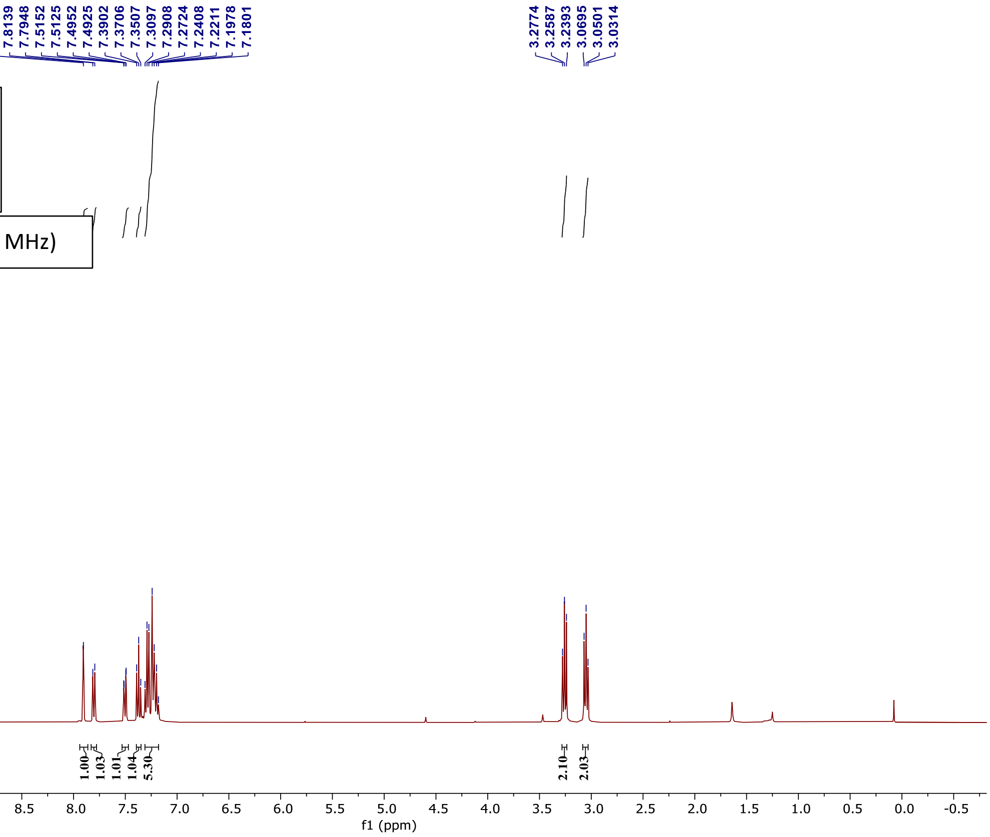
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz)

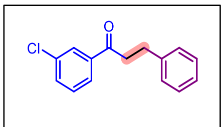

MeO
O
¹H NMR (CDCl₃, 400 MHz)


MeO
O
¹³C{¹H} NMR (CDCl₃, 100 MHz)

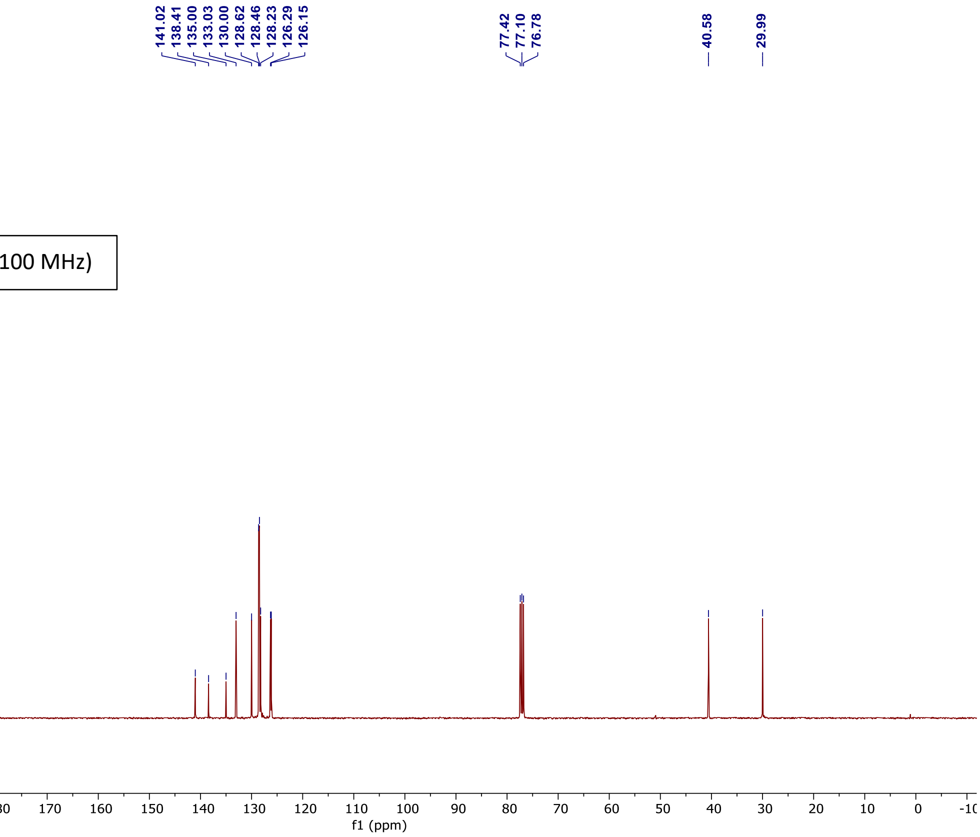


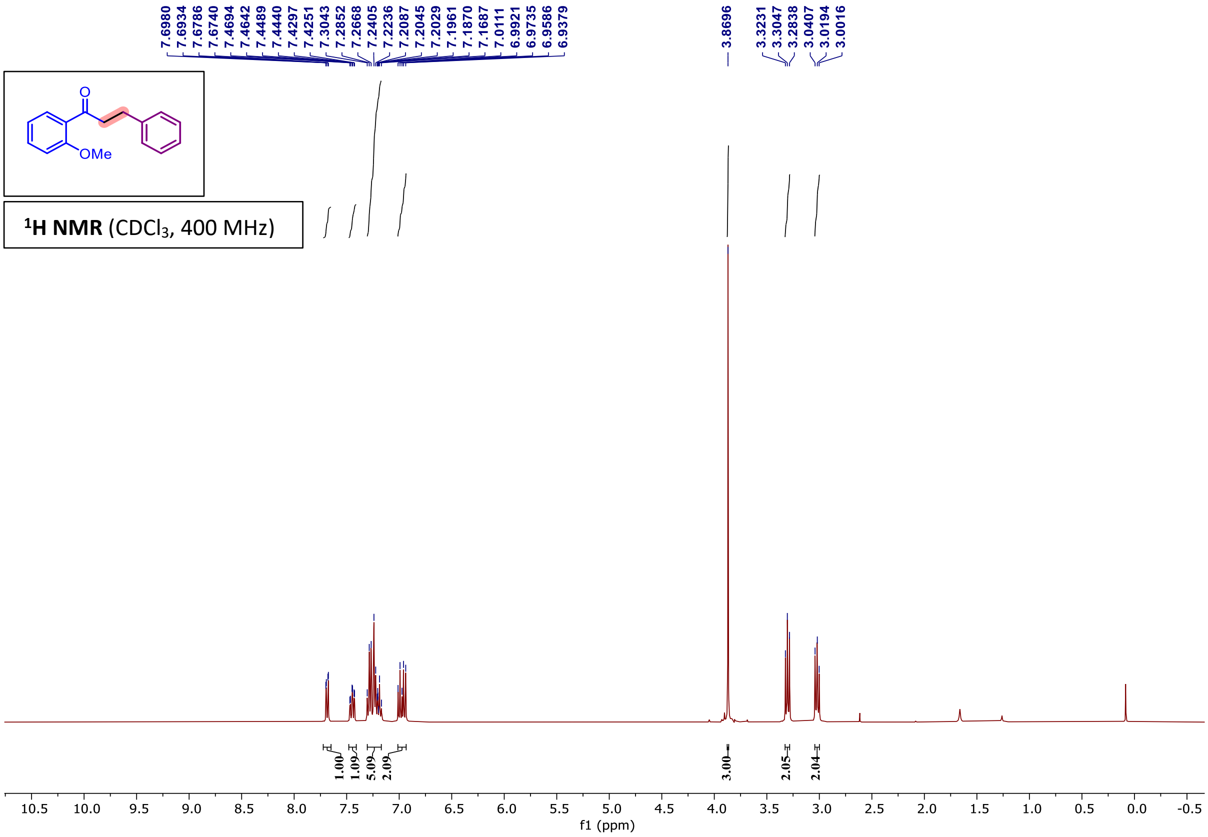
^{1}H NMR ($CDCl_3$, 400 MHz)

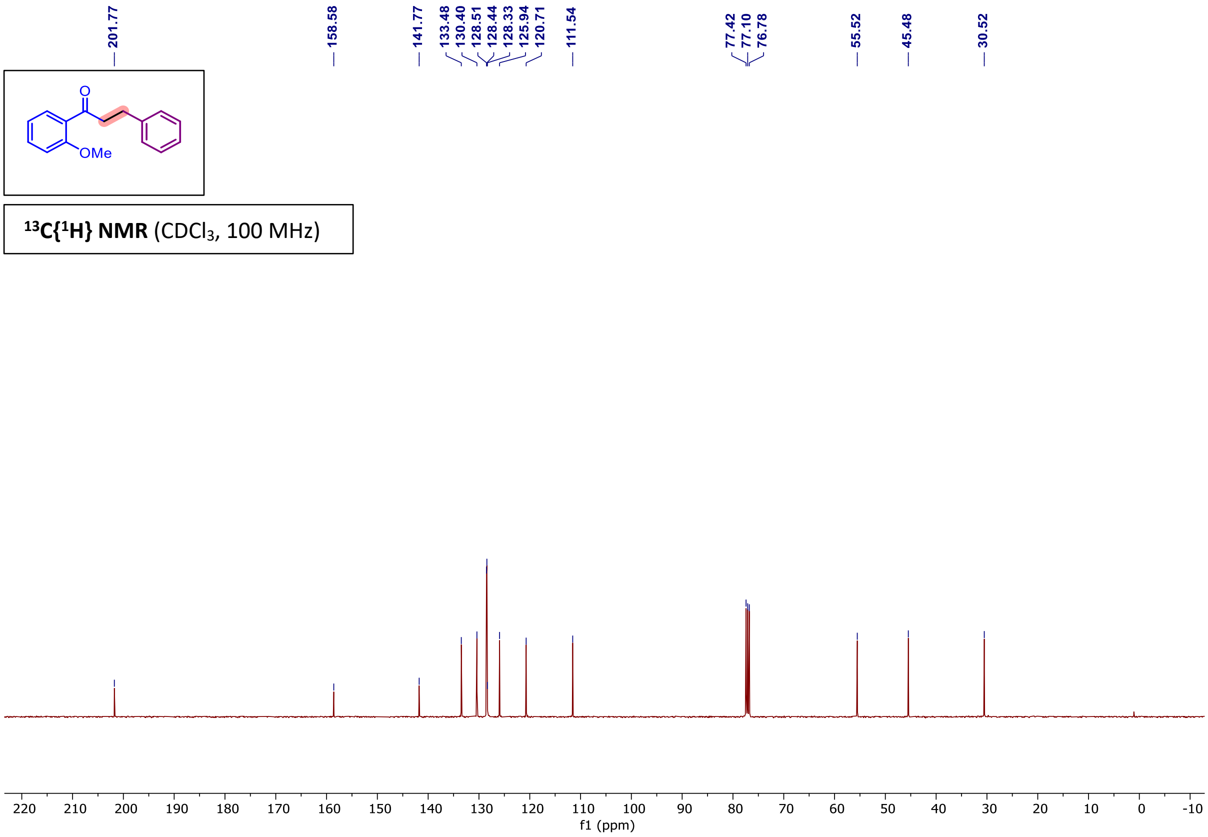


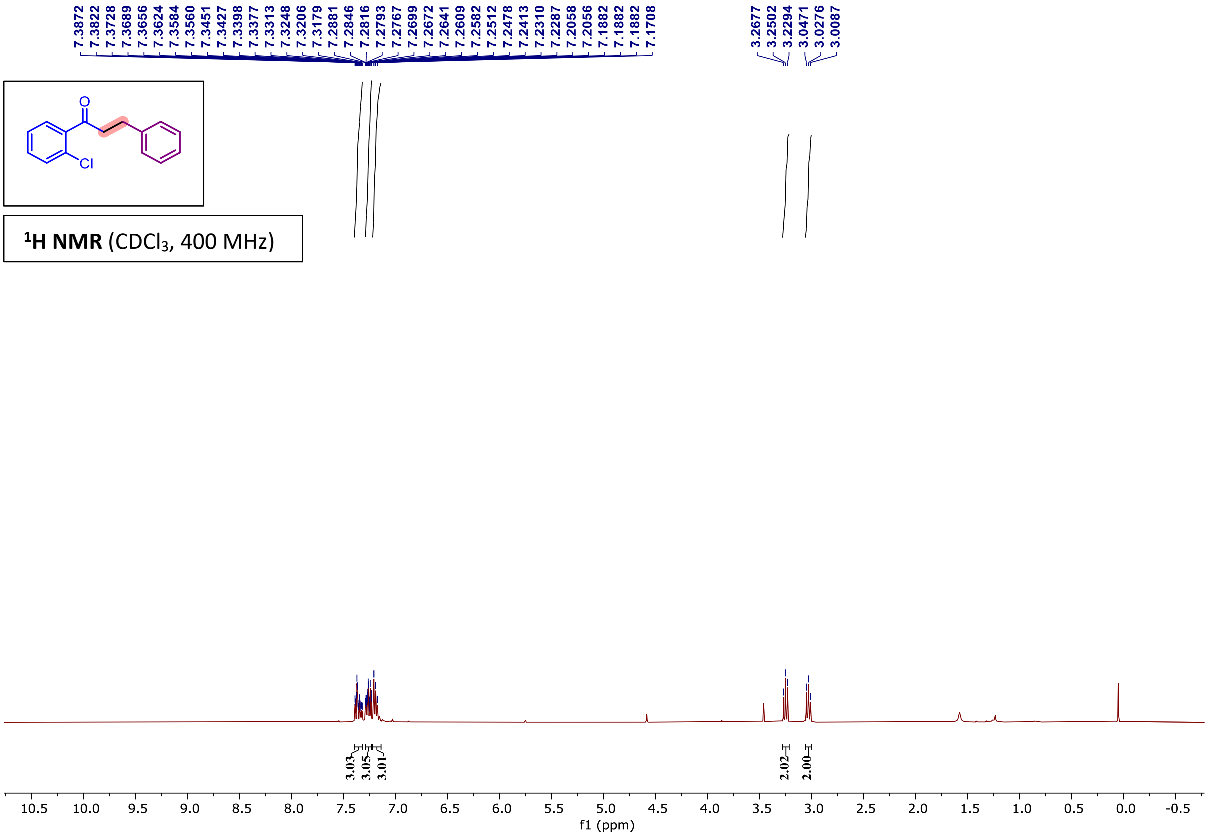


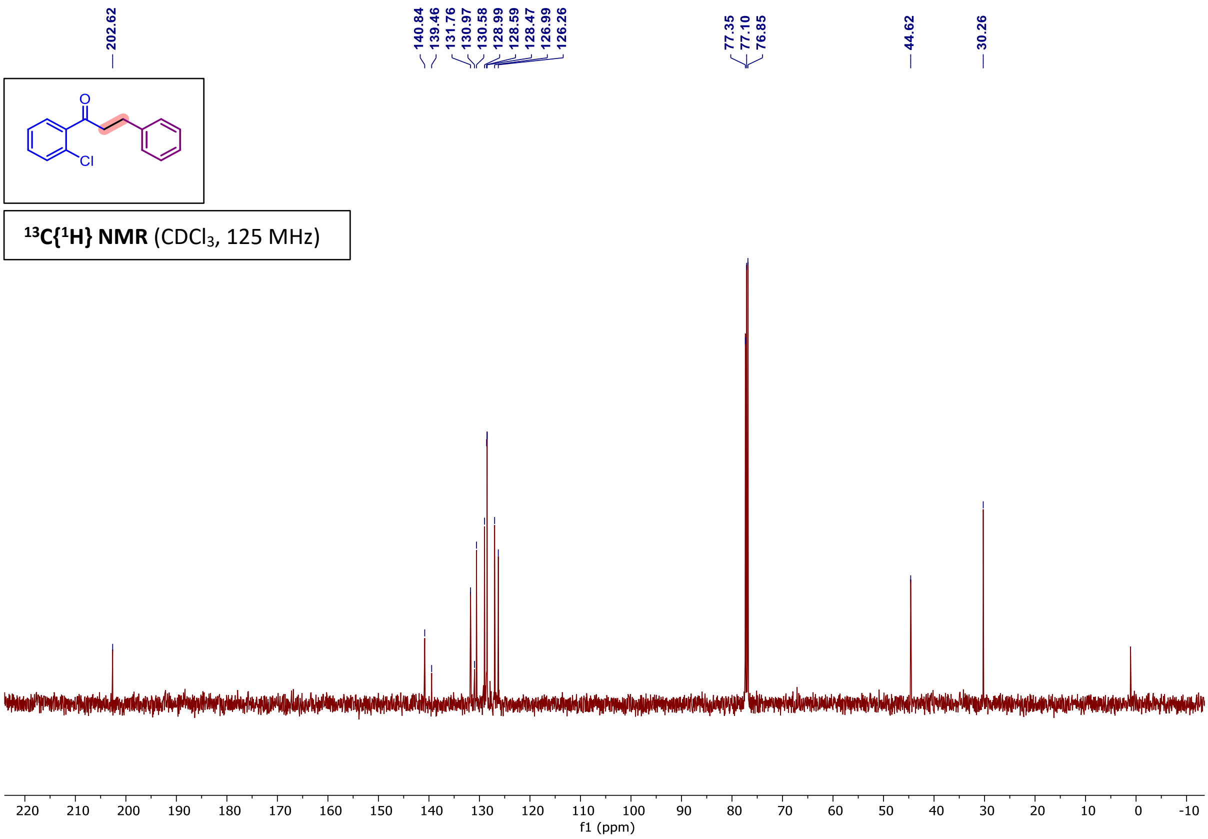
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)

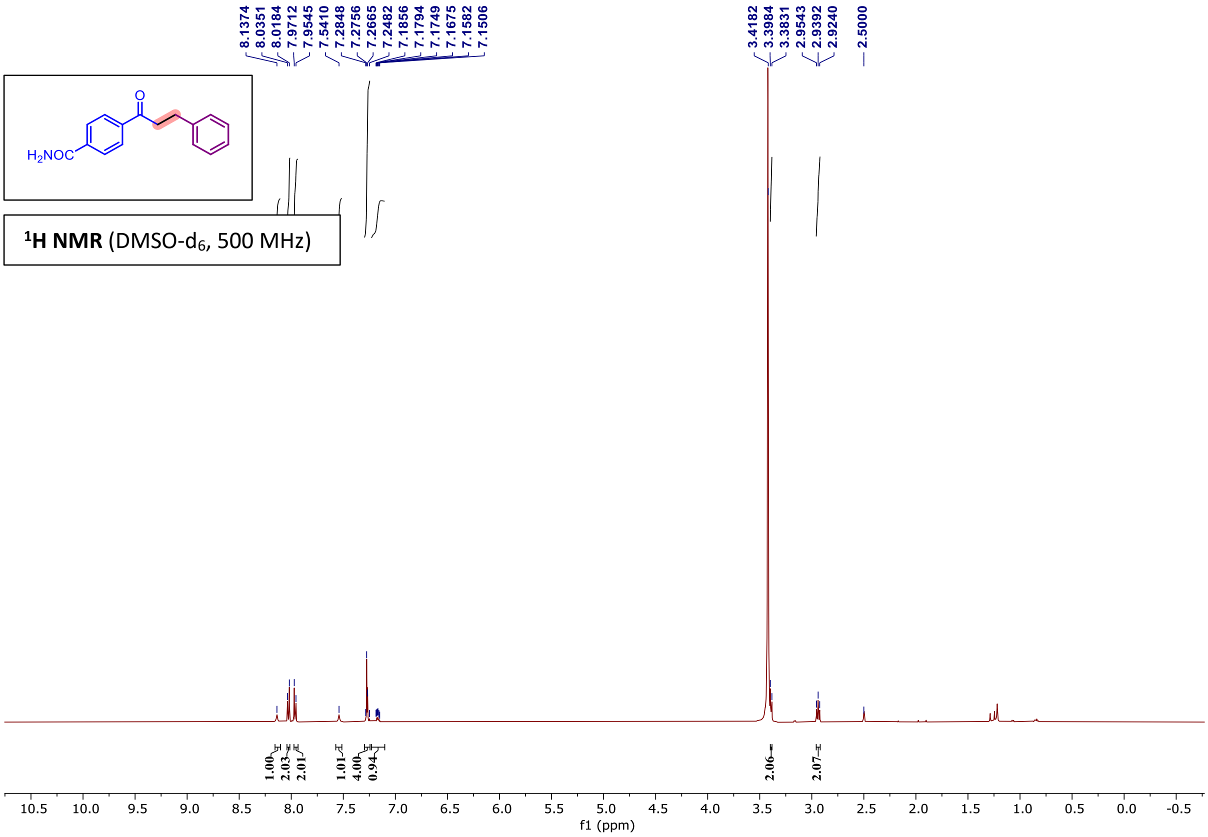



7.6980
7.6934
7.6786
7.6740
7.4694
7.4642
7.4489
7.4440
7.4297
7.4251
7.3043
7.2852
7.2668
7.2405
7.2236
7.2087
7.2045
7.2029
7.1961
7.1870
7.1687
7.0111
6.9921
6.9735
6.9586
6.9379
3.8696
3.3231
3.3047
3.2838
3.0407
3.0194
3.0016
O
OMe
¹H NMR (CDCl₃, 400 MHz)
1.00
1.09
5.09
2.09
3.00
2.05
2.04
f1 (ppm)

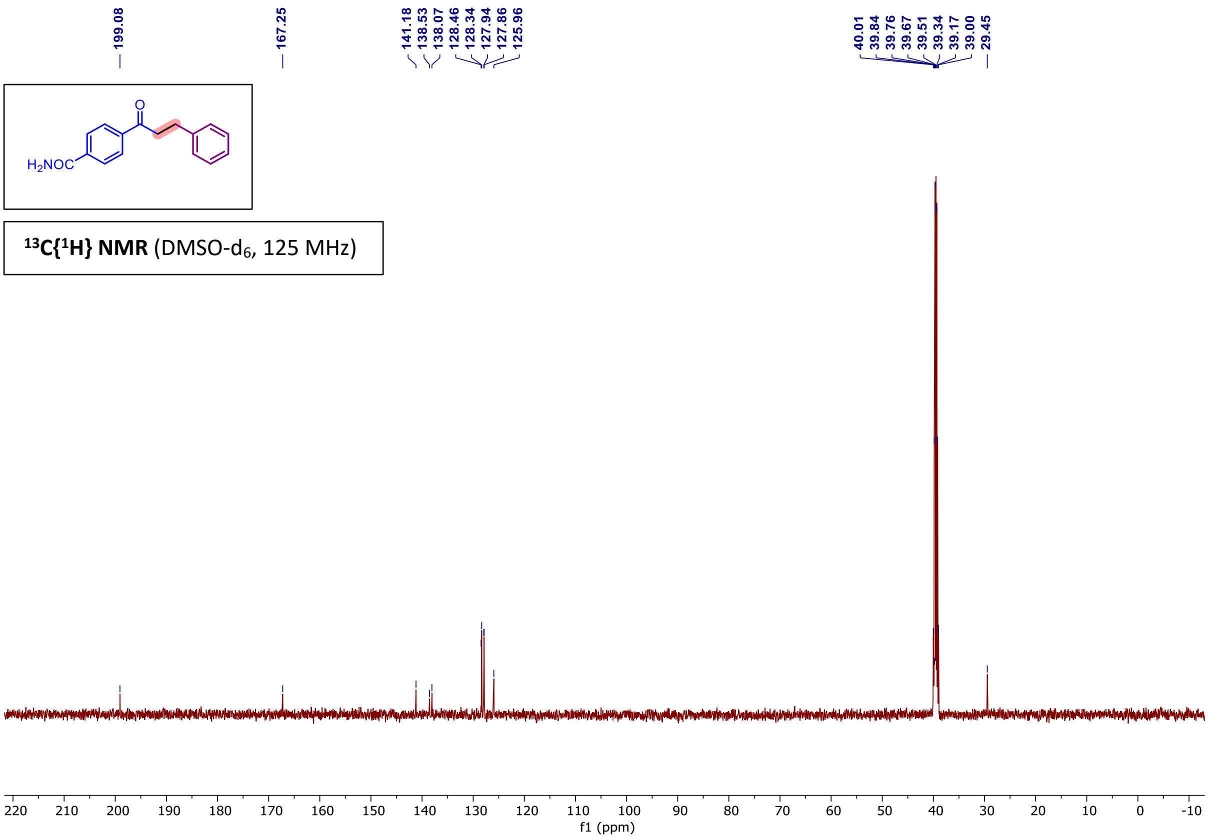

201.77
158.58
141.77
133.48
130.40
128.51
128.44
128.33
125.94
120.71
111.54
77.42
77.10
76.78
55.52
45.48
30.52
O
OMe
¹³C{¹H} NMR (CDCl₃, 100 MHz)
f1 (ppm)


7.3872
7.3822
7.3728
7.3689
7.3656
7.3624
7.3584
7.3560
7.3451
7.3427
7.3398
7.3377
7.3313
7.3248
7.3206
7.3179
7.2881
7.2846
7.2816
7.2793
7.2767
7.2699
7.2672
7.2641
7.2609
7.2582
7.2512
7.2478
7.2413
7.2310
7.2287
7.2058
7.2056
7.1882
7.1882
7.1708
3.2677
3.2502
3.2294
3.0471
3.0276
3.0087
O
Cl
¹H NMR (CDCl₃, 400 MHz)
3.03
3.05
3.01
2.02
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

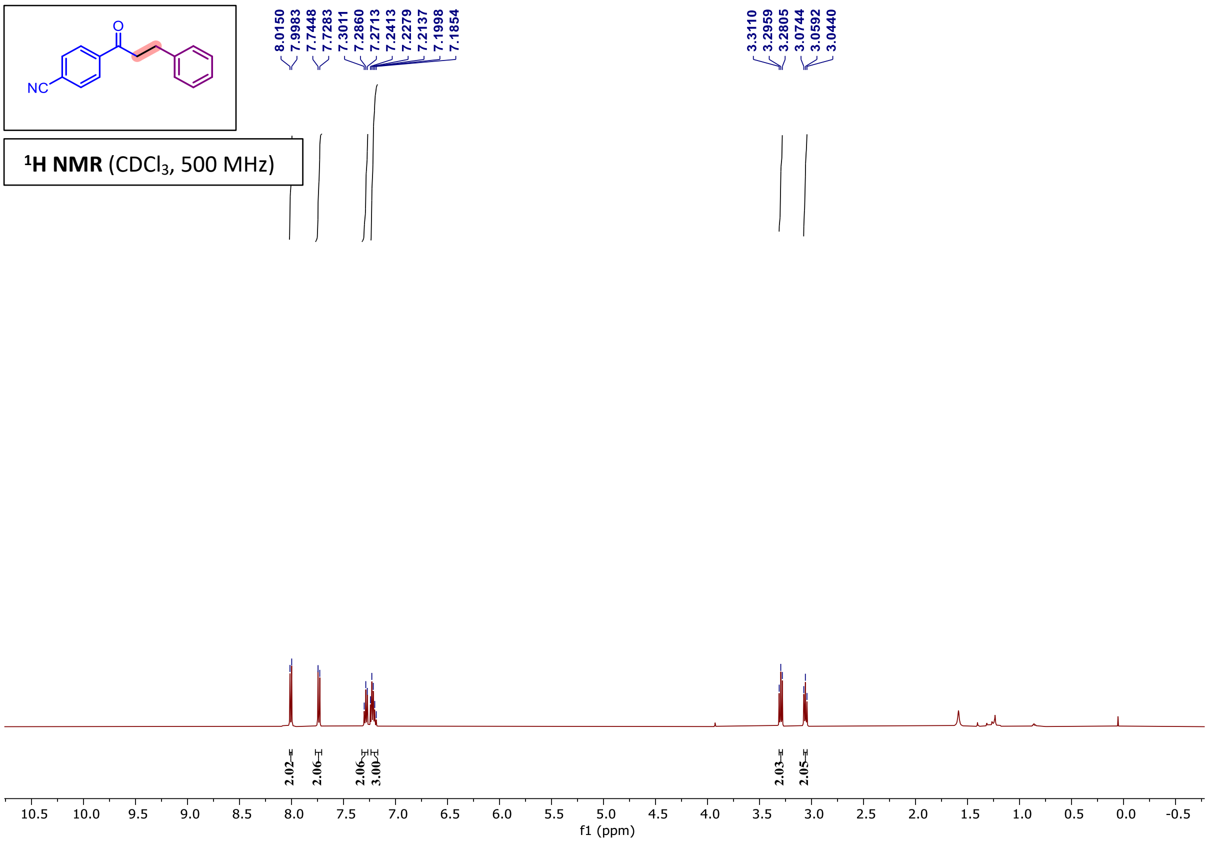

202.62
140.84
139.46
131.76
130.97
130.58
128.99
128.59
128.47
126.99
126.26
77.35
77.10
76.85
44.62
30.26
O
Cl
¹³C{¹H} NMR (CDCl₃, 125 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



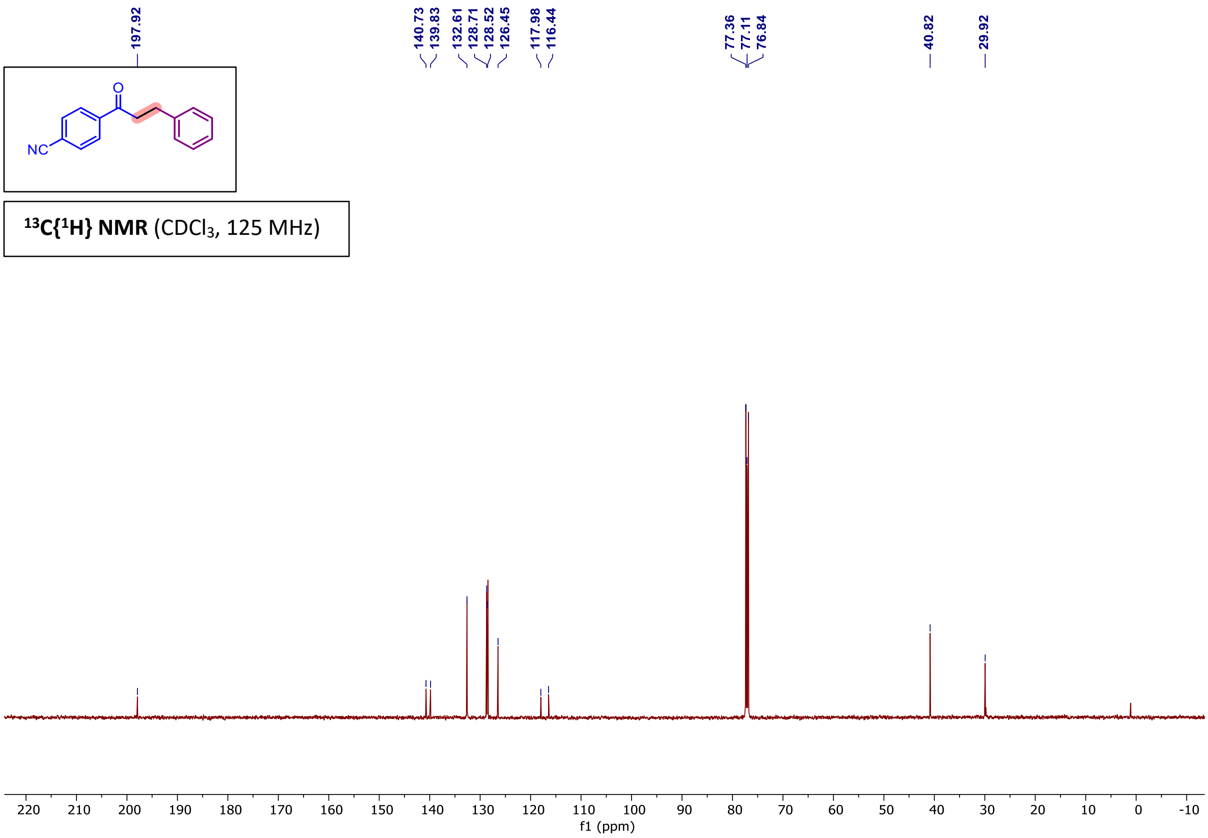
^{1}H NMR (DMSO-d$_6$, 500 MHz)



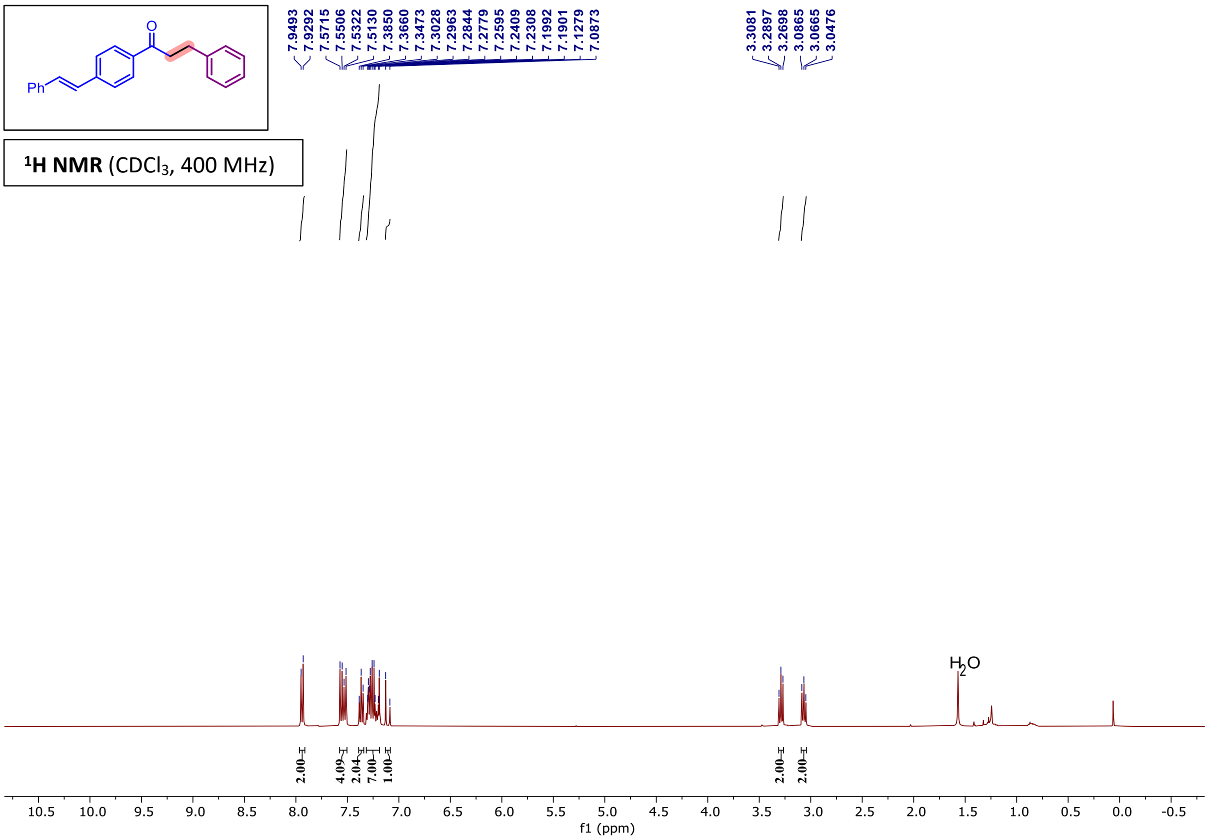
^{13}C{^{1}H} NMR (DMSO-d$_6$, 125 MHz)

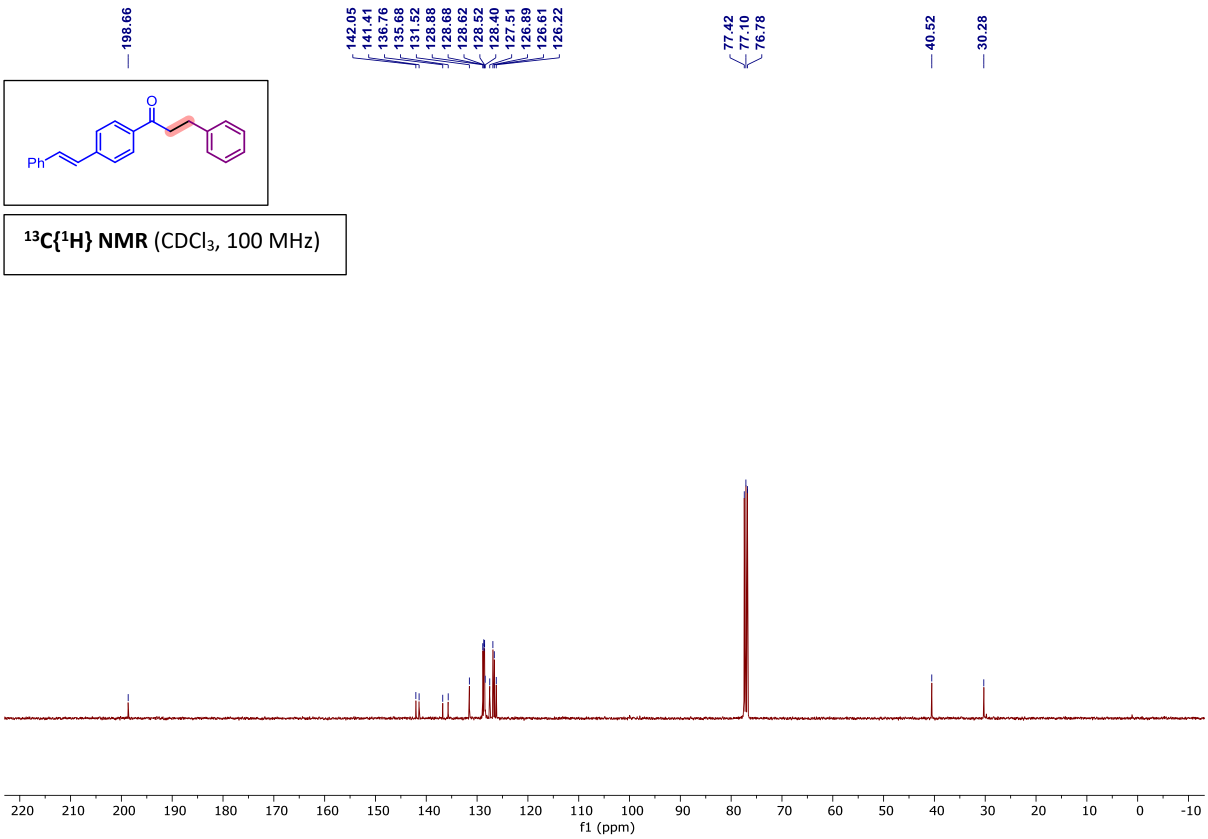


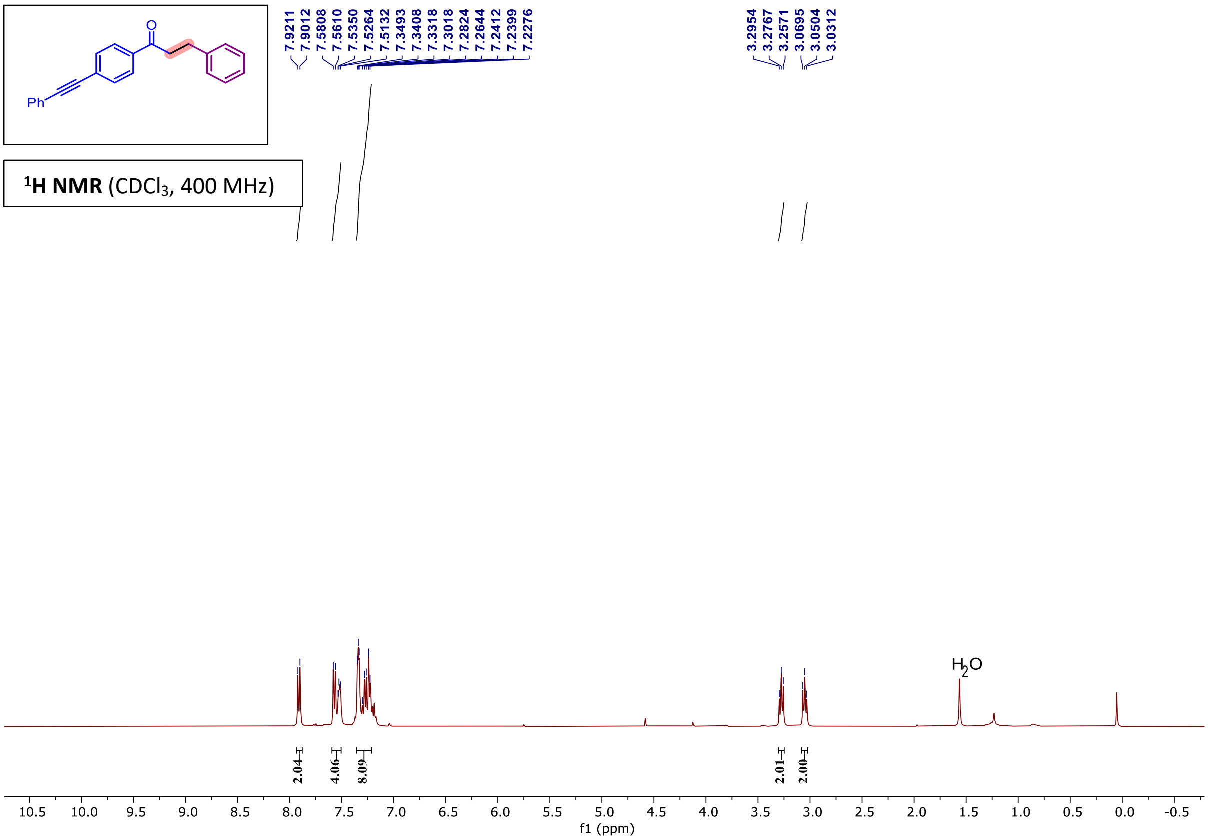
^{1}H NMR ($CDCl_3$, 500 MHz)



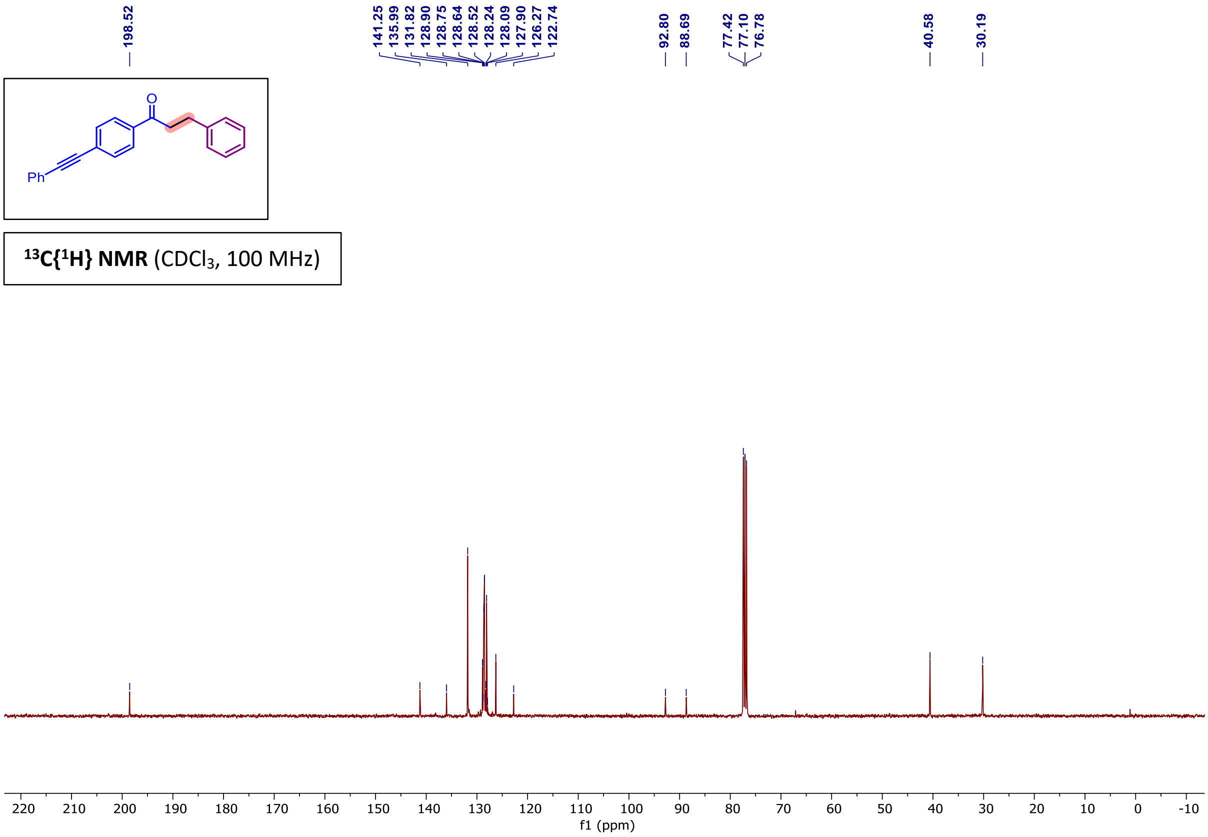
^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)


Ph
O
¹H NMR (CDCl3, 400 MHz)
7.9493 7.9292 7.5715 7.5506 7.5322 7.5130 7.3850 7.3660 7.3473 7.3028 7.2963 7.2844 7.2779 7.2595 7.2409 7.2308 7.1992 7.1901 7.1279 7.0873
3.3081 3.2897 3.2698 3.0865 3.0665 3.0476
H2O
2.00 4.09 2.04 7.00 1.00 2.00 2.00
f1 (ppm)

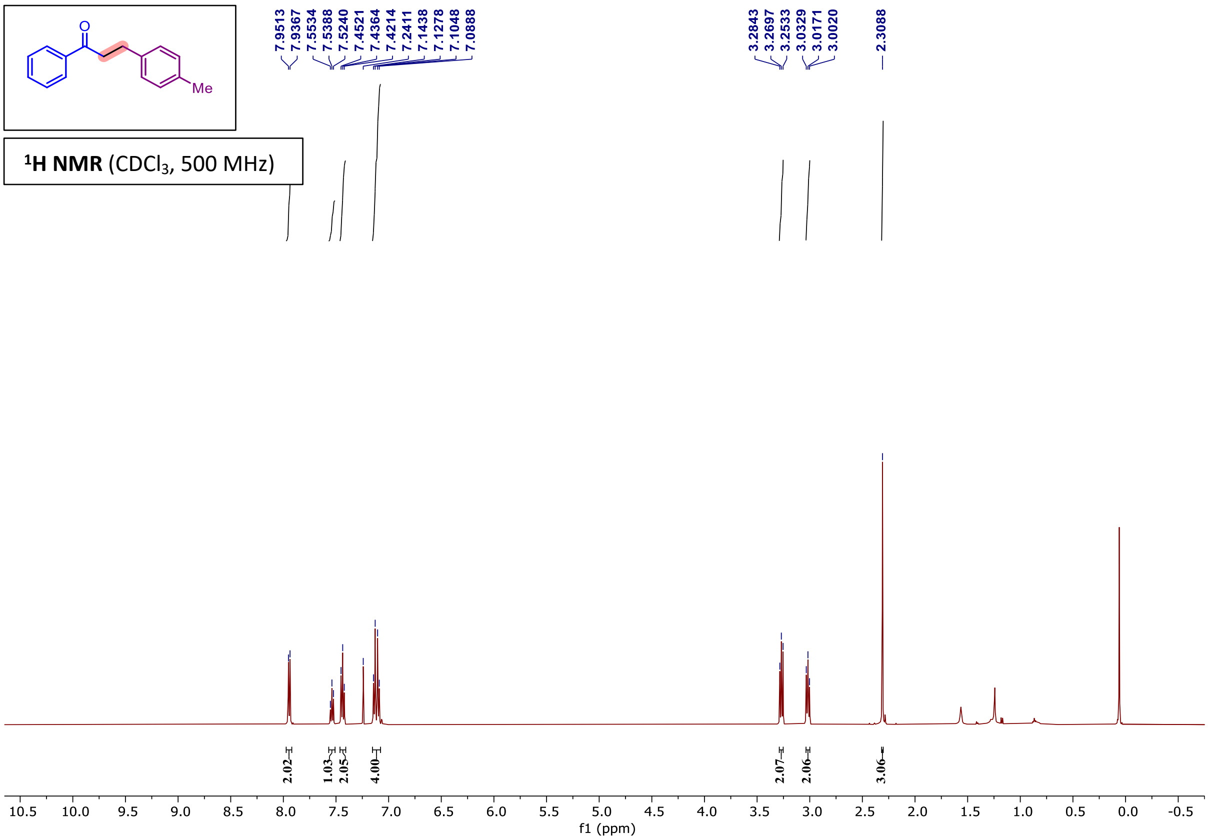

198.66
142.05 141.41 136.76 135.68 131.52 128.88 128.68 128.62 128.52 128.40 127.51 126.89 126.61 126.22
77.42 77.10 76.78
40.52
30.28
Ph
O
¹³C{¹H} NMR (CDCl3, 100 MHz)
f1 (ppm)

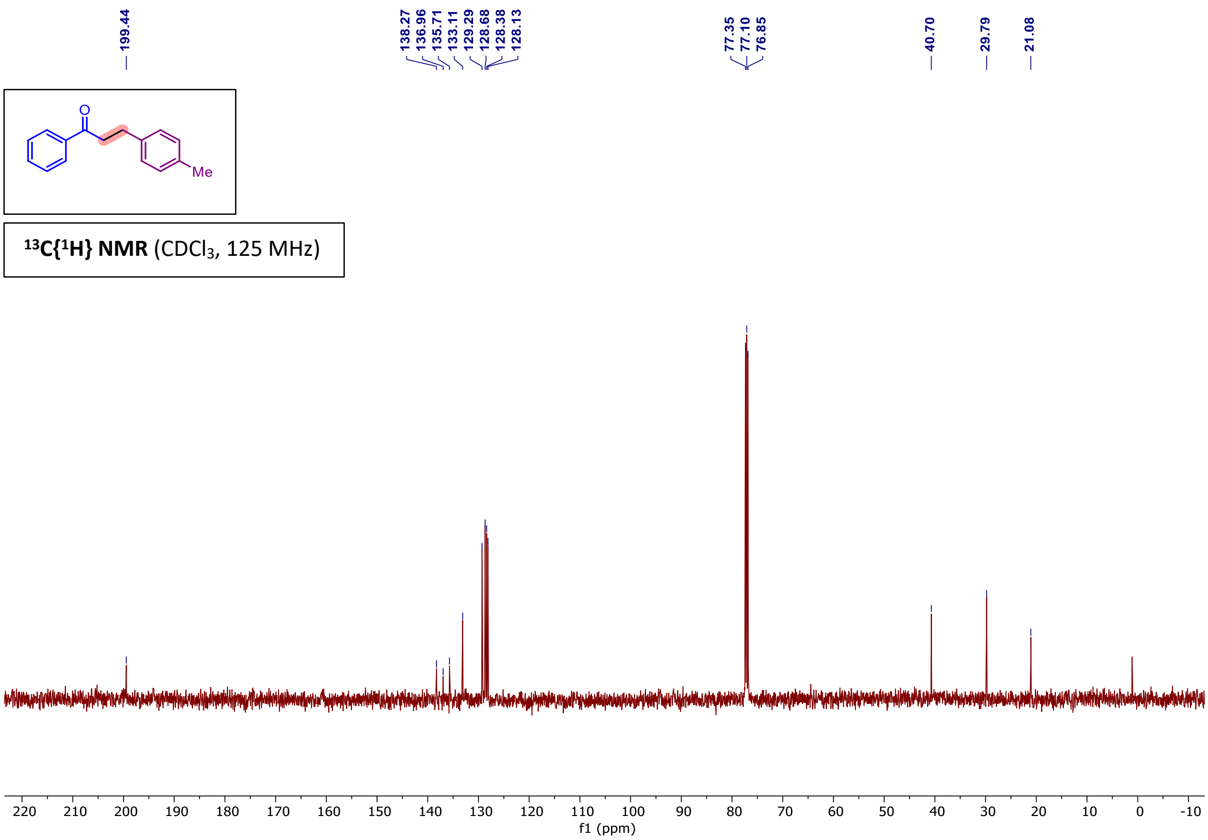


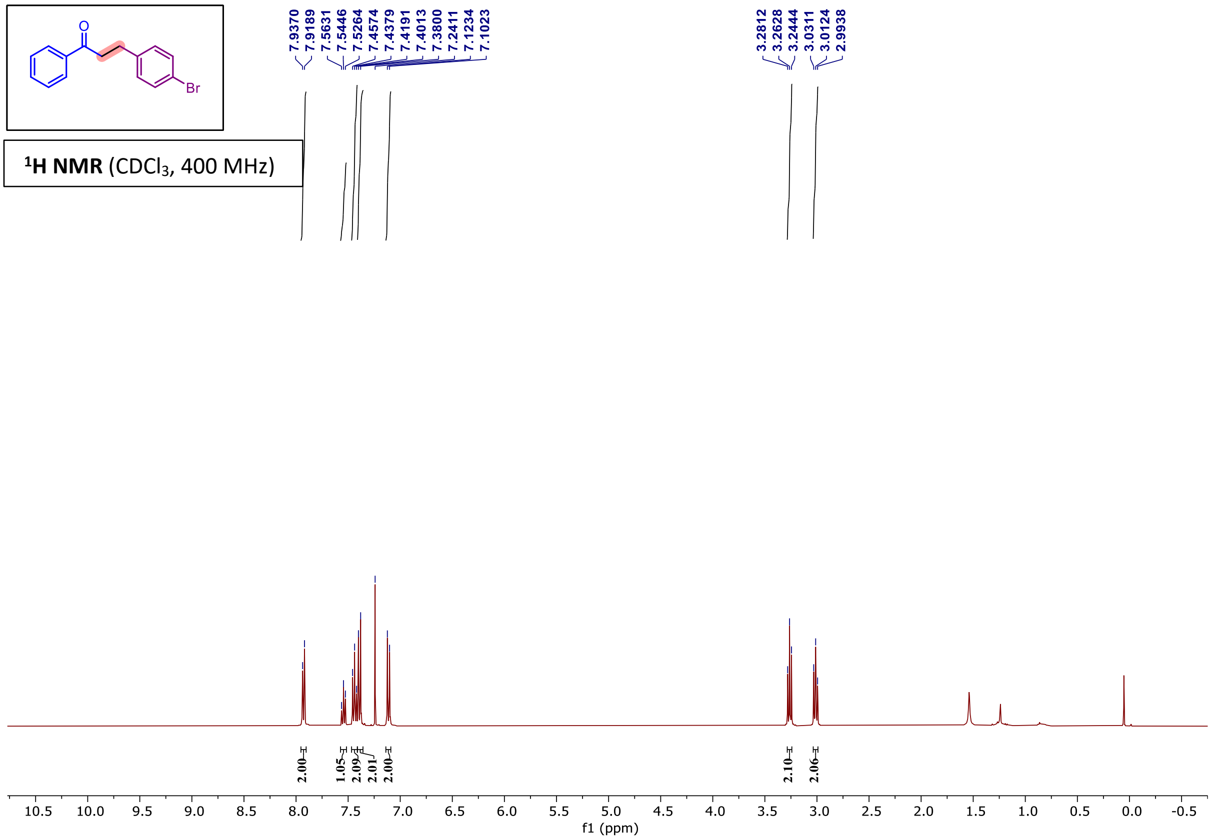
[1]H NMR ($CDCl_3$, 400 MHz)

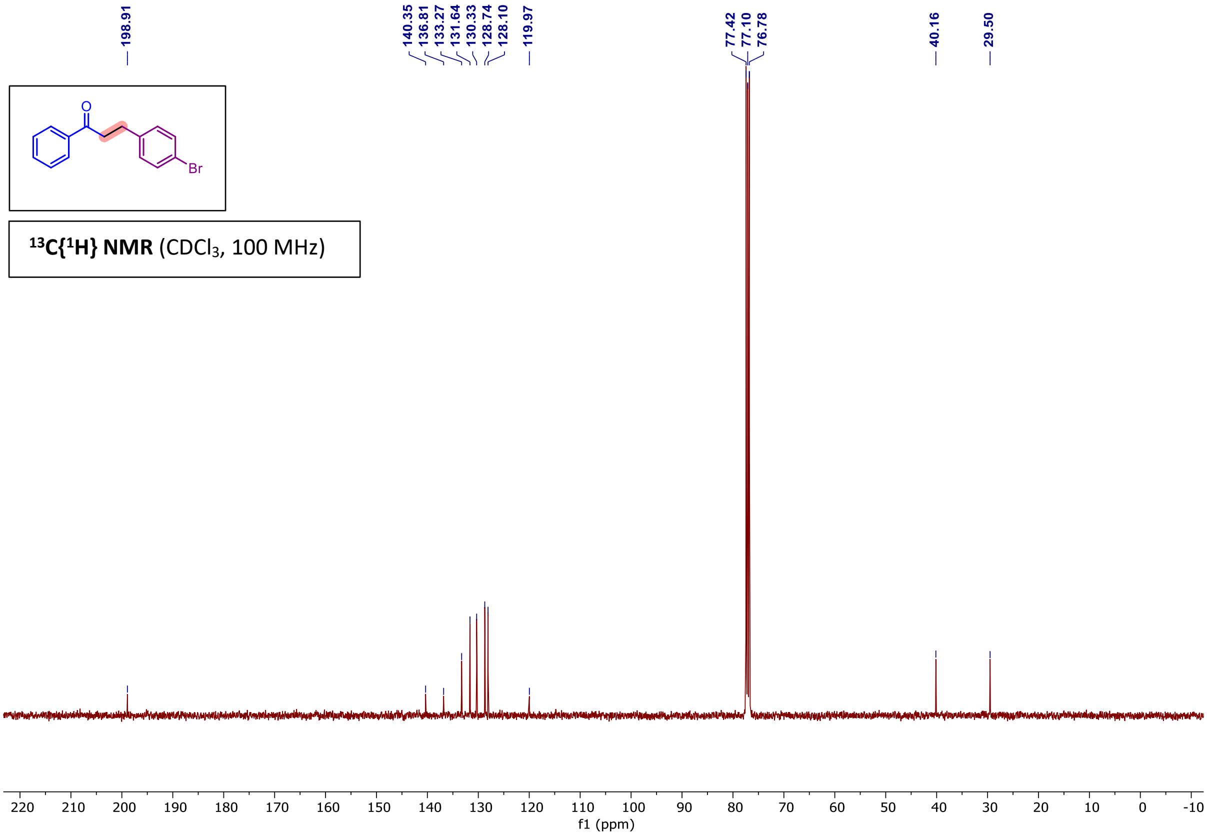


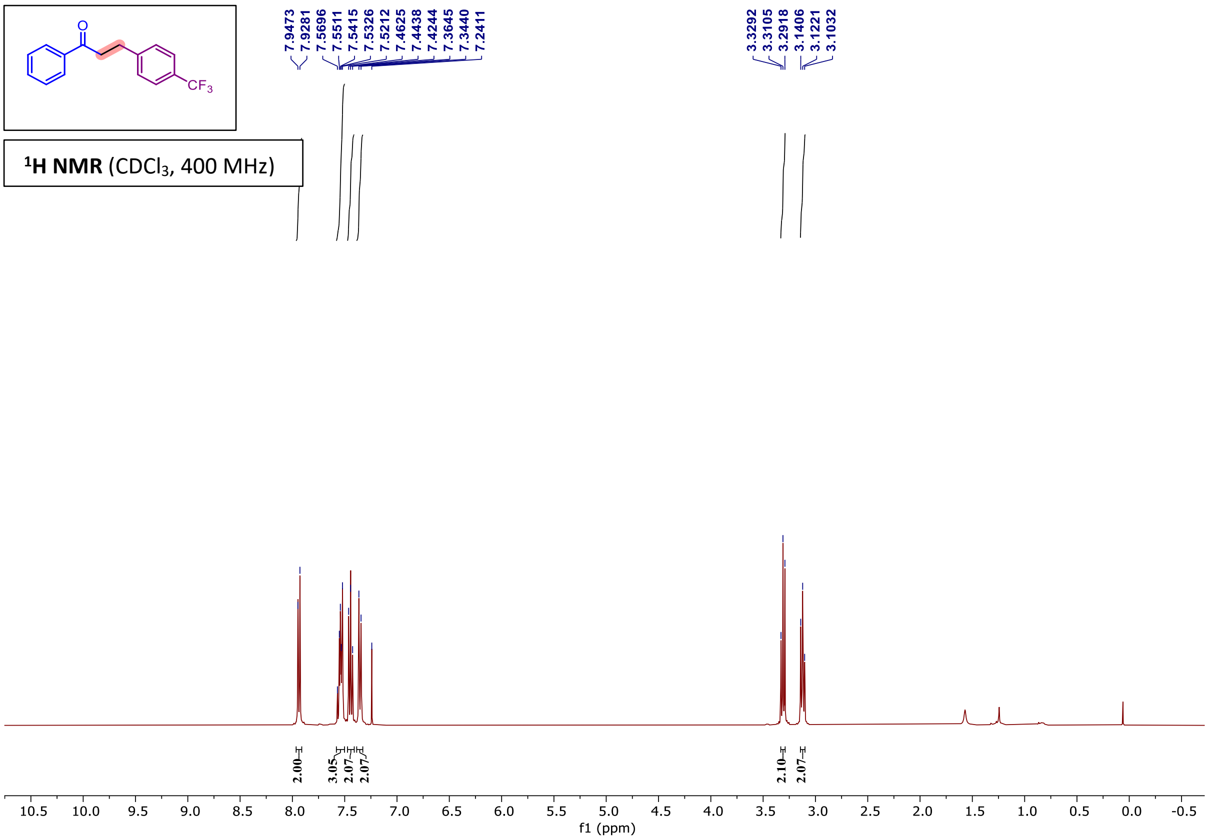
[13]C{[1]H} NMR ($CDCl_3$, 100 MHz)

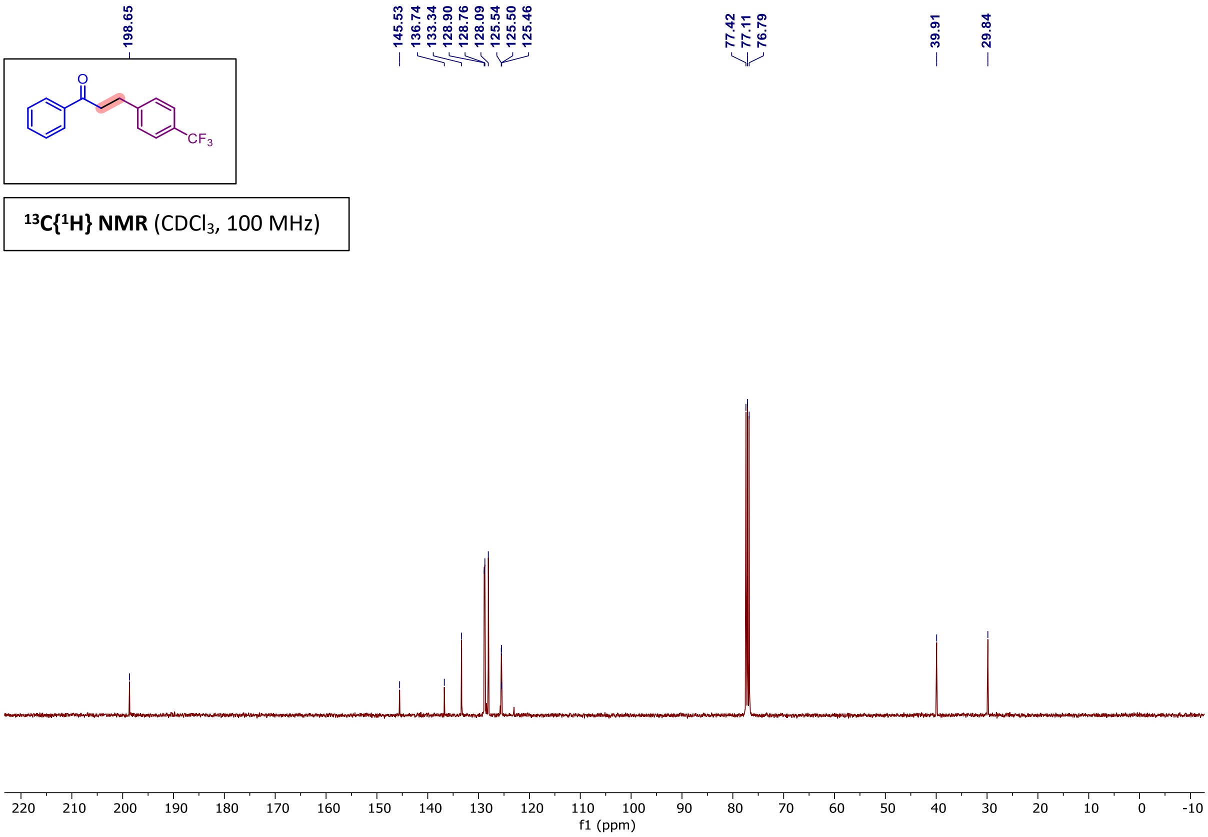

O
Me
¹H NMR (CDCl₃, 500 MHz)
7.9513
7.9367
7.5534
7.5388
7.5240
7.4521
7.4364
7.4214
7.2411
7.1438
7.1278
7.1048
7.0888
3.2843
3.2697
3.2533
3.0329
3.0171
3.0020
2.3088
2.02
1.03
2.05
4.00
2.07
2.06
3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

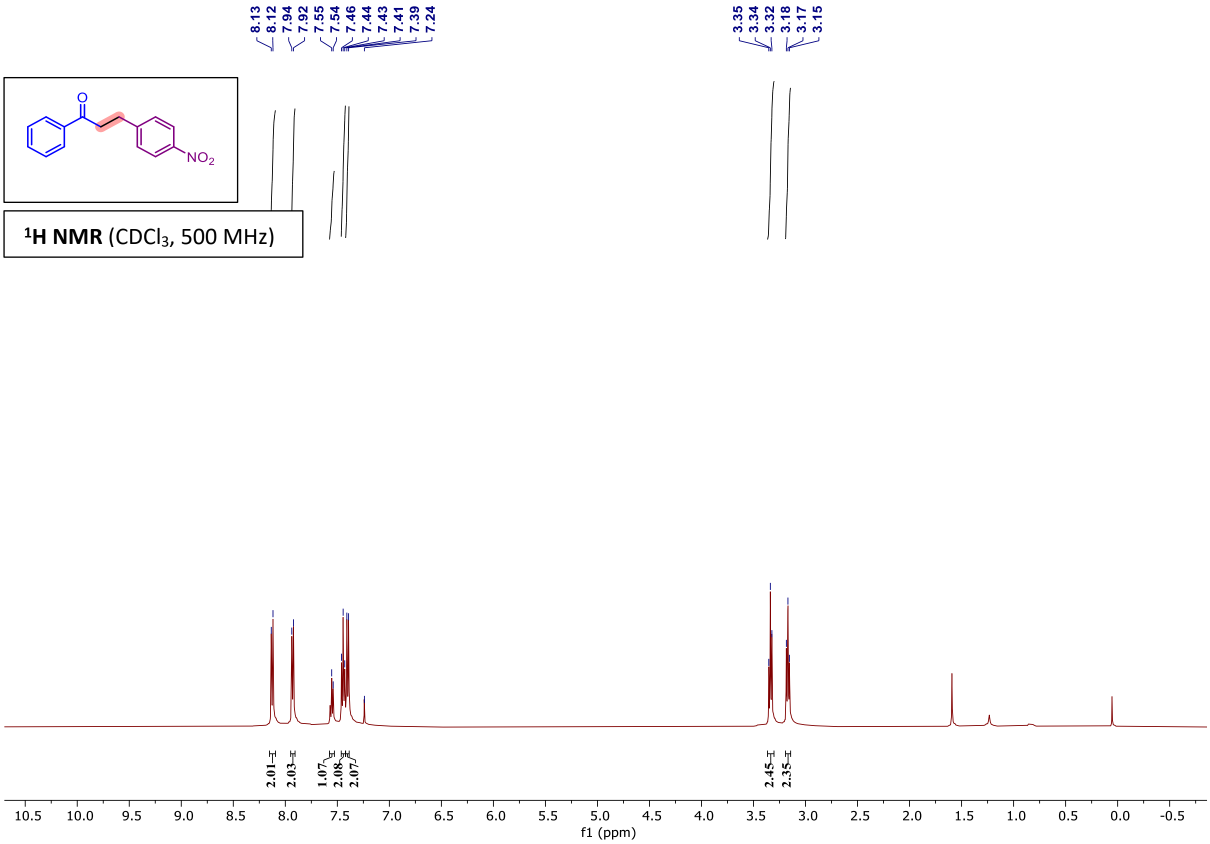

199.44
138.27
136.96
135.71
133.11
129.29
128.68
128.38
128.13
77.35
77.10
76.85
40.70
29.79
21.08
O
Me
¹³C{¹H} NMR (CDCl₃, 125 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
Br
¹H NMR (CDCl₃, 400 MHz)
7.9370
7.9189
7.5631
7.5446
7.5264
7.4574
7.4379
7.4191
7.4013
7.3800
7.2411
7.1234
7.1023
3.2812
3.2628
3.2444
3.0311
3.0124
2.9938
2.00
1.05
2.09
2.01
2.00
2.10
2.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

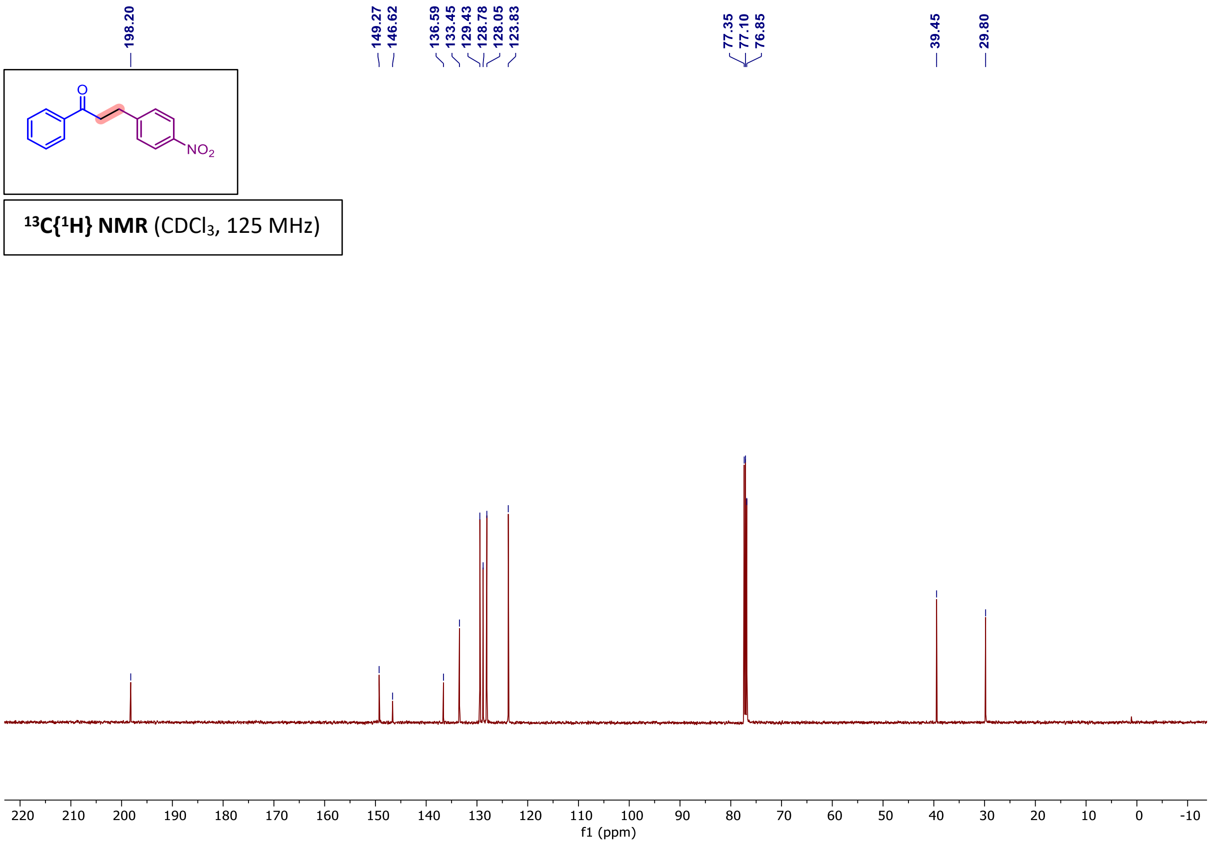

198.91
140.35
136.81
133.27
131.64
130.33
128.74
128.10
119.97
77.42
77.10
76.78
40.16
29.50
O
Br
¹³C{¹H} NMR (CDCl₃, 100 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
CF3
1H NMR (CDCl3, 400 MHz)
7.9473
7.9281
7.5696
7.5511
7.5415
7.5326
7.5212
7.4625
7.4438
7.4244
7.3645
7.3440
7.2411
3.3292
3.3105
3.2918
3.1406
3.1221
3.1032
2.00
3.05
2.07
2.07
2.10
2.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

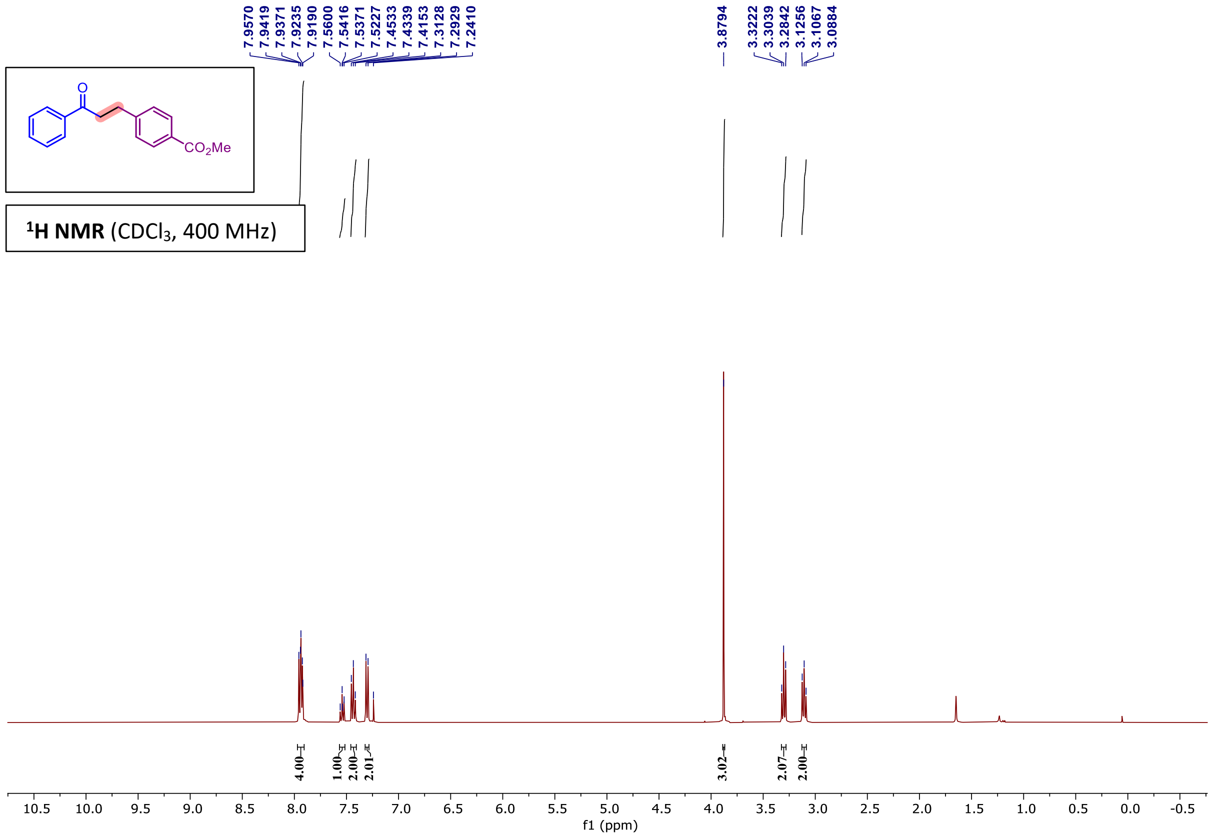

198.65
145.53
136.74
133.34
128.90
128.76
128.09
125.54
125.50
125.46
77.42
77.11
76.79
39.91
29.84
O
CF3
13C{1H} NMR (CDCl3, 100 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

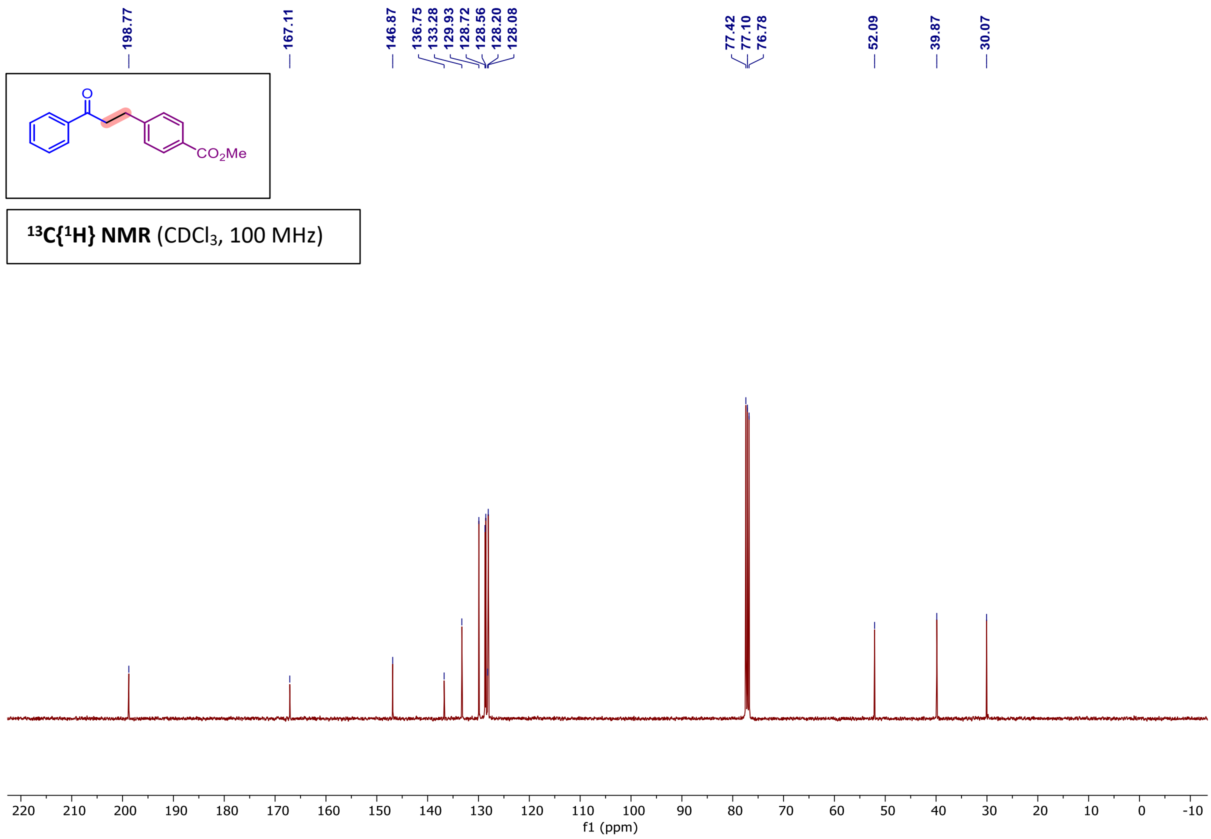


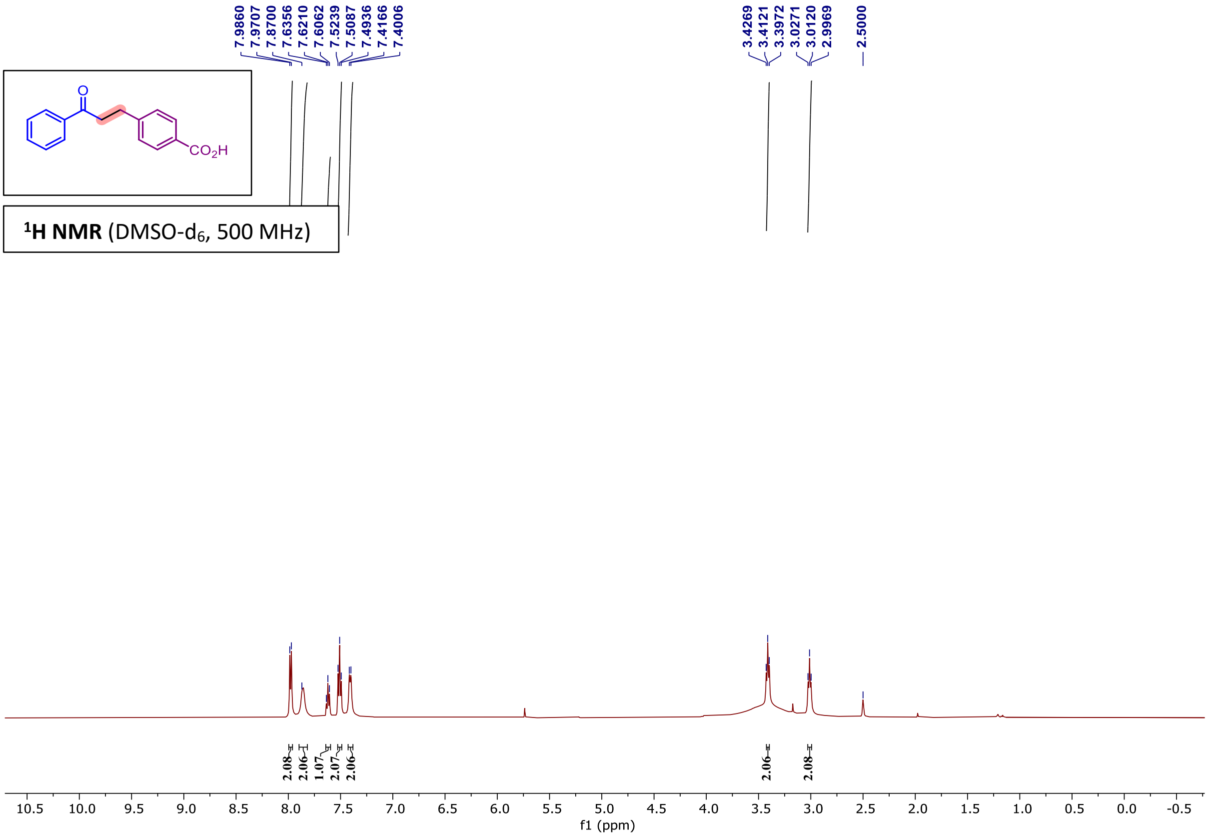
NO_2
^{1}H NMR ($CDCl_3$, 500 MHz)
8.13 8.12 7.94 7.92 7.55 7.54 7.46 7.44 7.43 7.41 7.39 7.24
3.35 3.34 3.32 3.18 3.17 3.15
2.01 2.03 1.07 2.08 2.07 2.45 2.35
f1 (ppm)



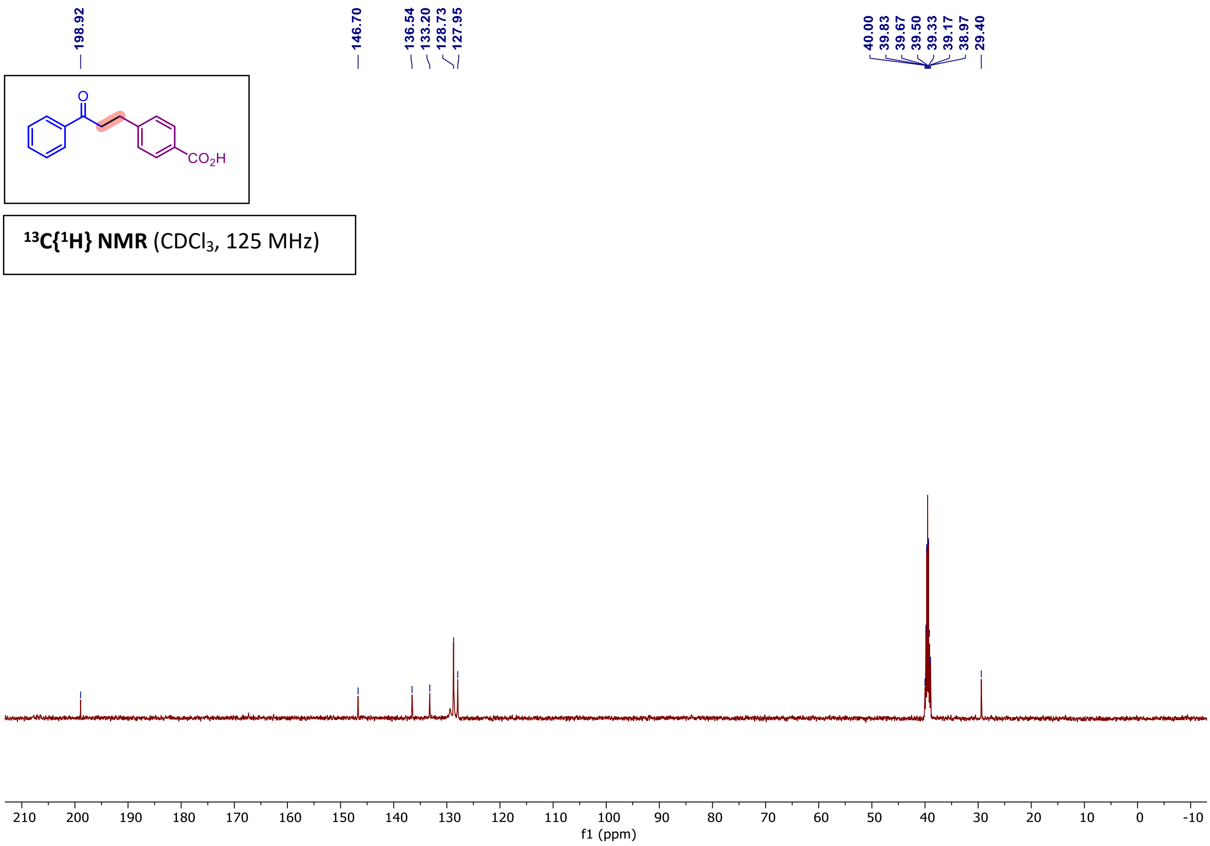
NO_2
^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)
198.20
149.27 146.62
136.59 133.45 129.43 128.78 128.05 123.83
77.35 77.10 76.85
39.45
29.80
f1 (ppm)


CO2Me
1H NMR (CDCl3, 400 MHz)
7.9570
7.9419
7.9371
7.9235
7.9190
7.5600
7.5416
7.5371
7.5227
7.4533
7.4339
7.4153
7.3128
7.2929
7.2410
3.8794
3.3222
3.3039
3.2842
3.1256
3.1067
3.0884
4.00
1.00
2.00
2.01
3.02
2.07
2.00
f1 (ppm)

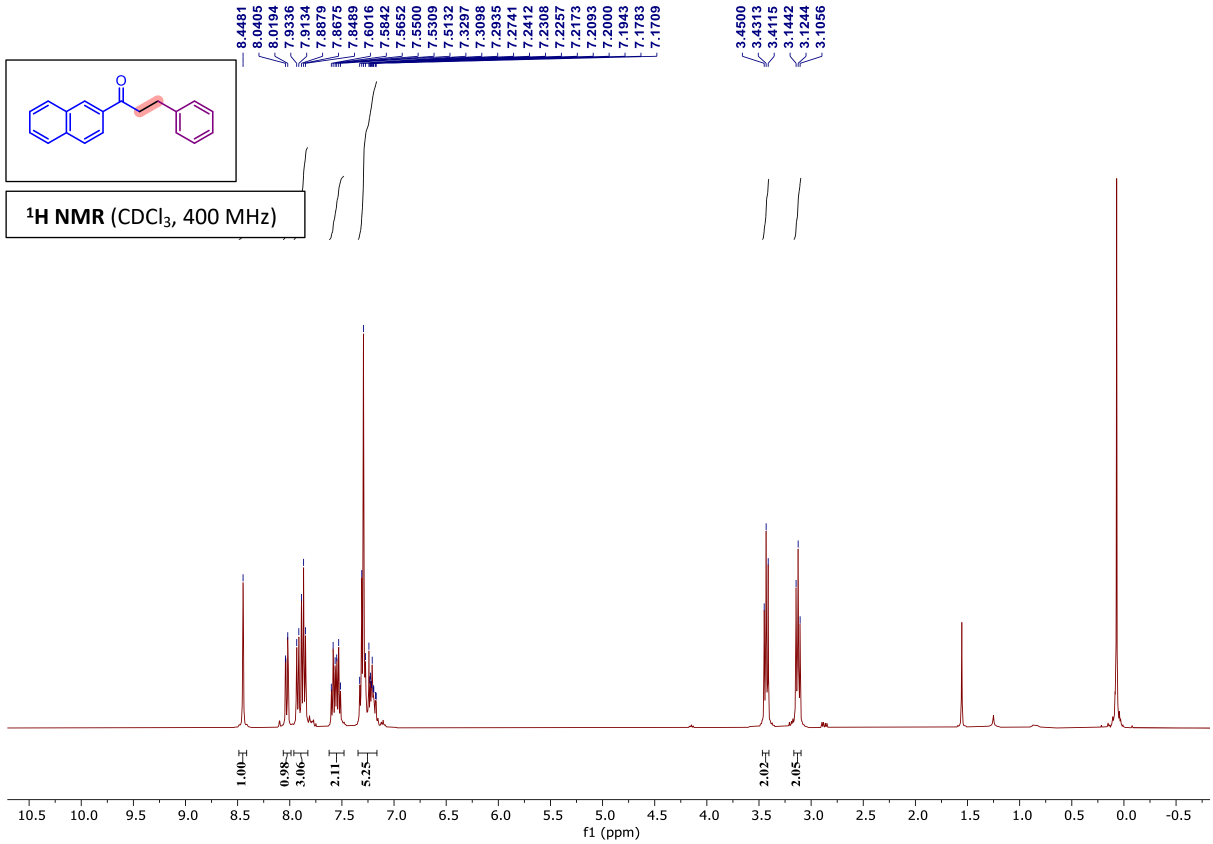

CO2Me
13C{1H} NMR (CDCl3, 100 MHz)
198.77
167.11
146.87
136.75
133.28
129.93
128.72
128.56
128.20
128.08
77.42
77.10
76.78
52.09
39.87
30.07
f1 (ppm)

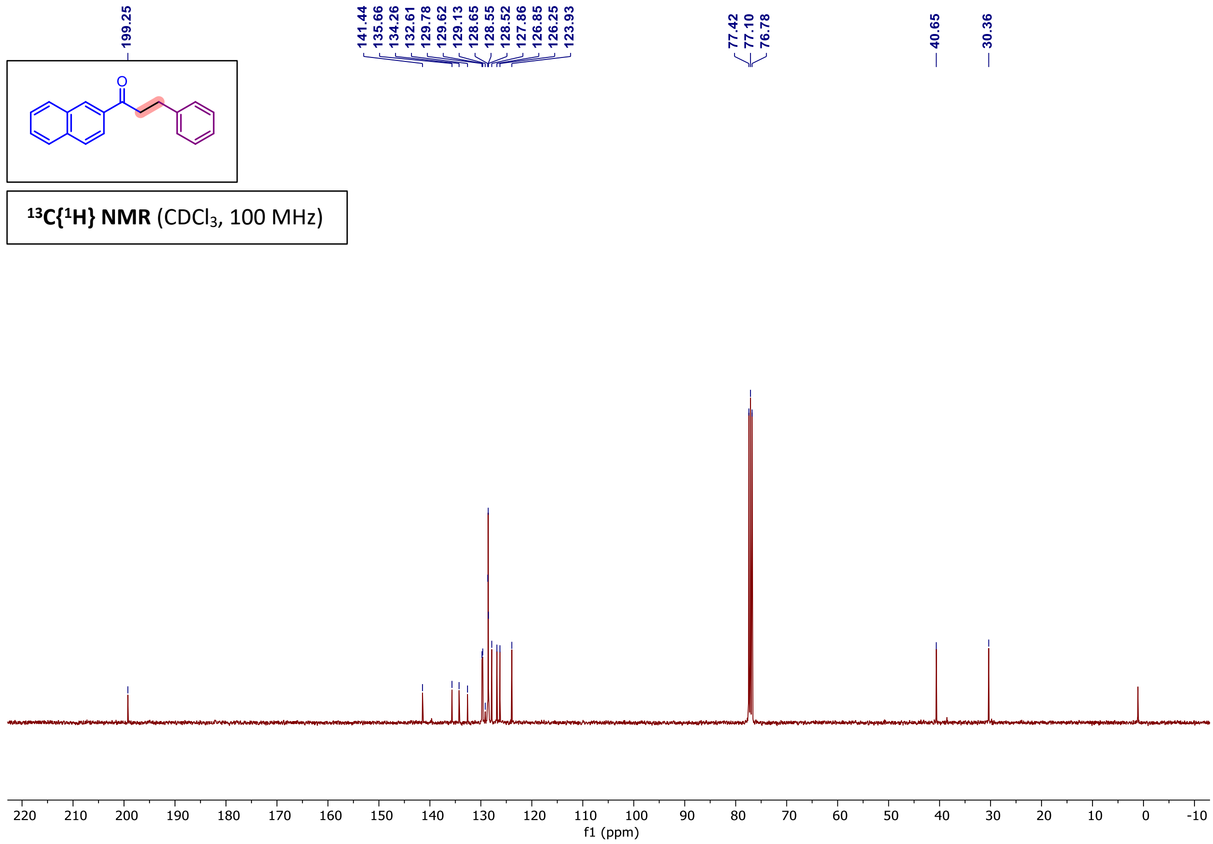


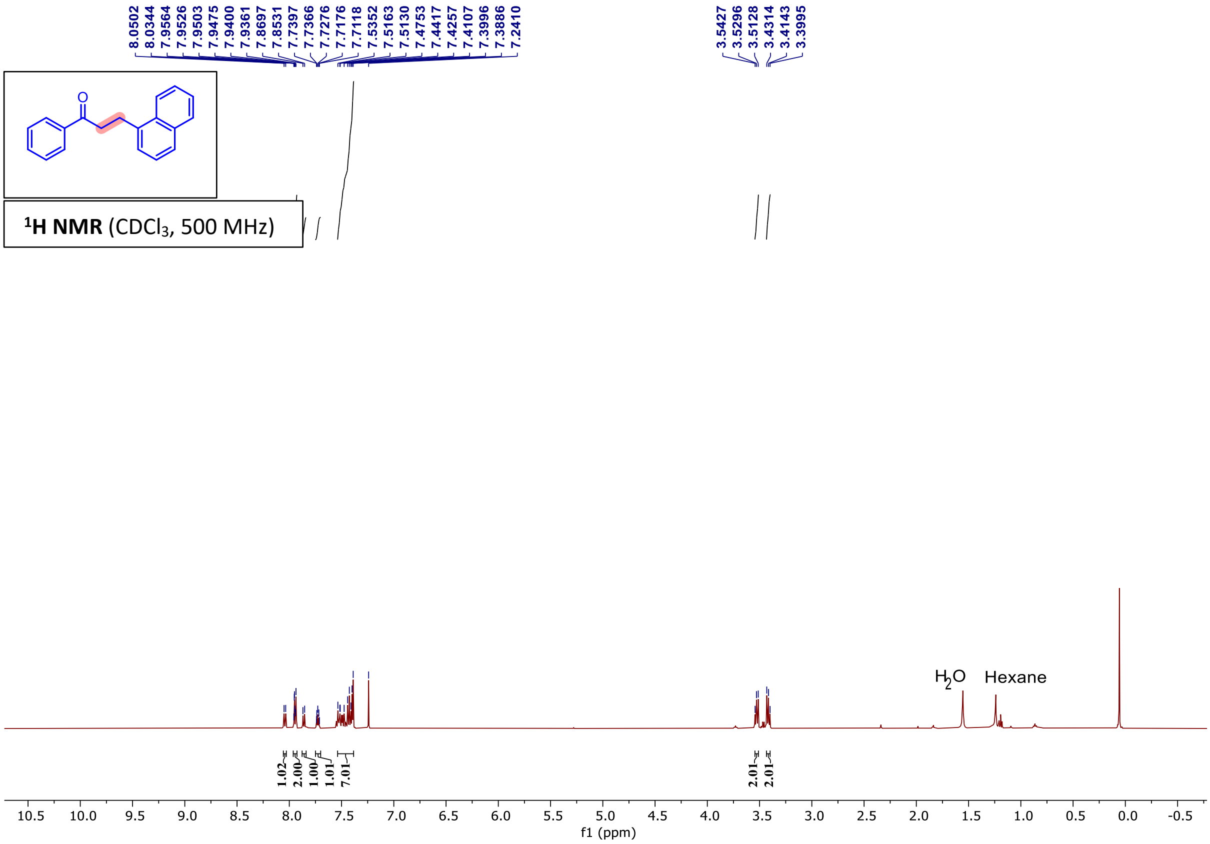
^{1}H NMR (DMSO-d$_6$, 500 MHz)

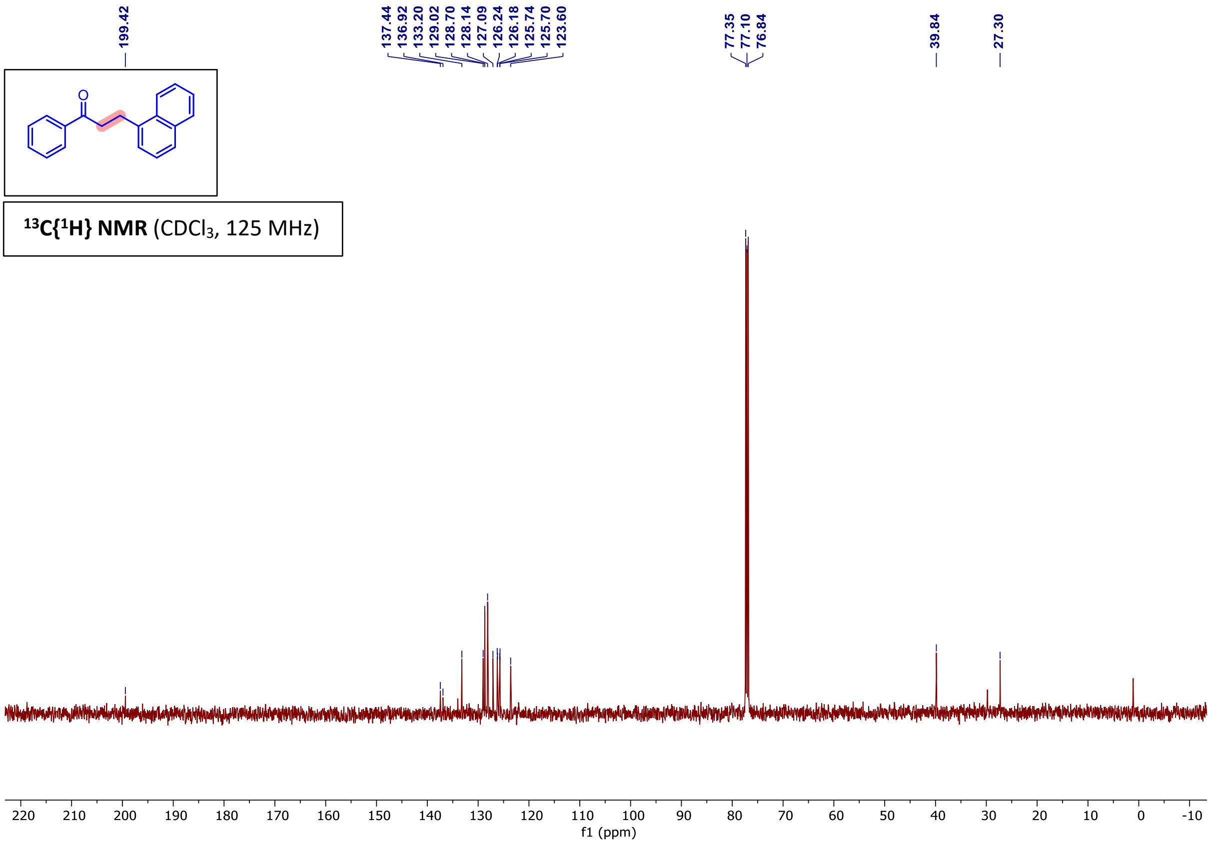


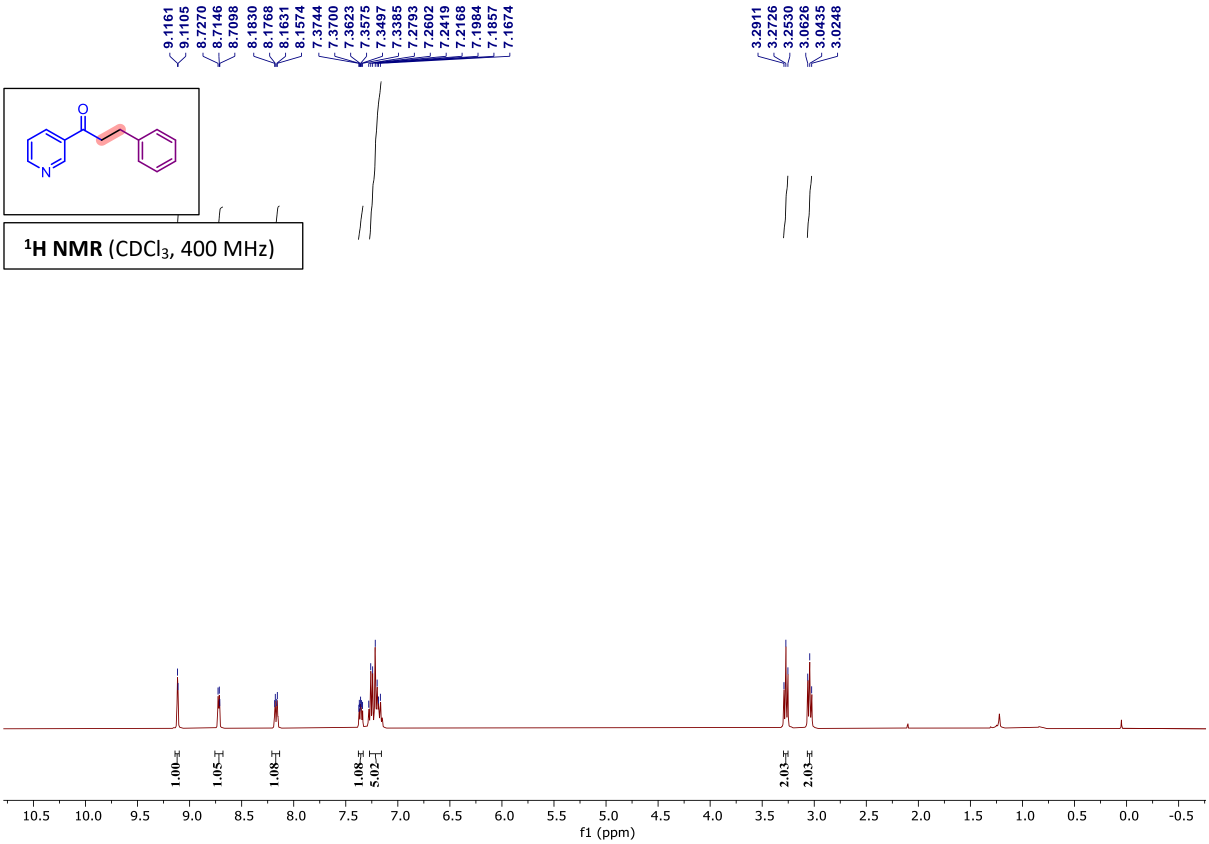
^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)

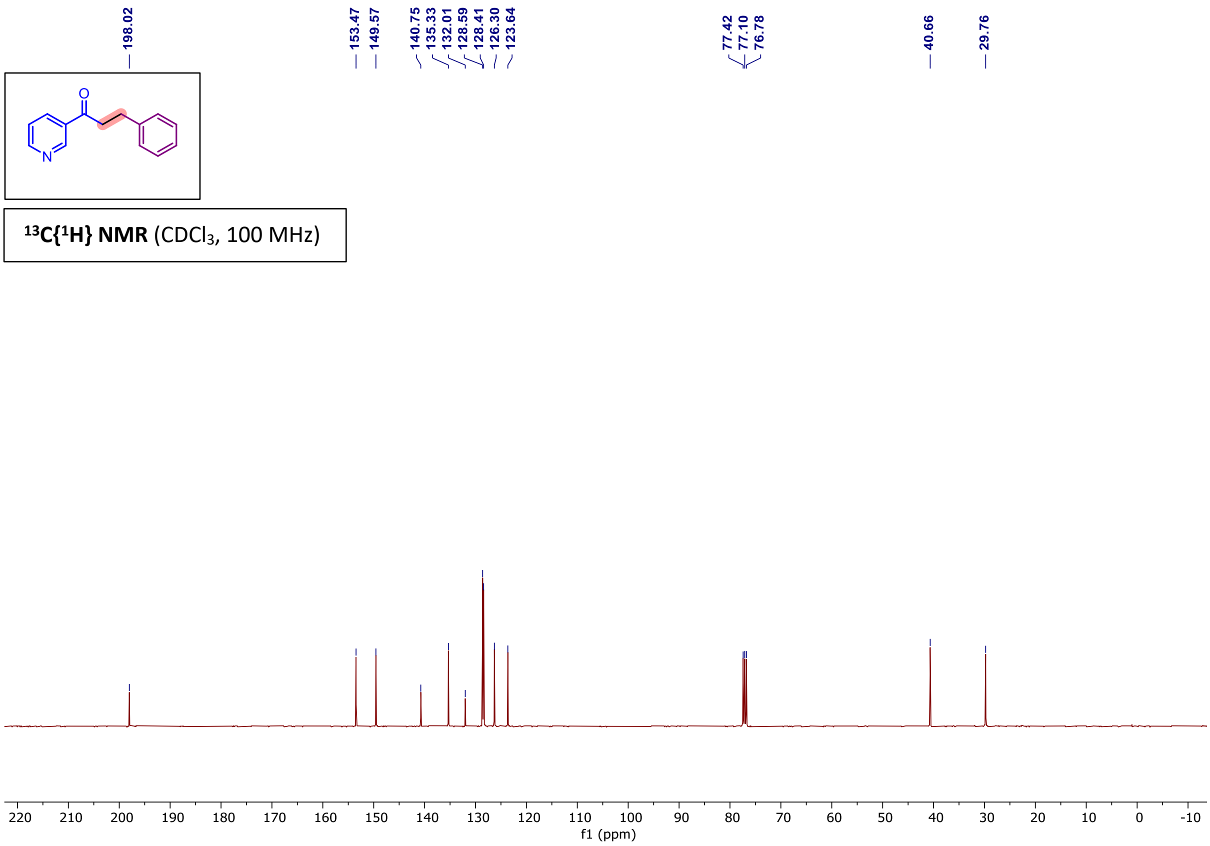

O
¹H NMR (CDCl₃, 400 MHz)
8.4481 8.0405 8.0194 7.9336 7.9134 7.8879 7.8675 7.8489 7.6016 7.5842 7.5652 7.5500 7.5309 7.5132 7.3297 7.3098 7.2935 7.2741 7.2412 7.2308 7.2257 7.2173 7.2093 7.2000 7.1943 7.1783 7.1709
3.4500 3.4313 3.4115 3.1442 3.1244 3.1056
1.00 0.98 3.06 2.11 5.25 2.02 2.05
f1 (ppm)

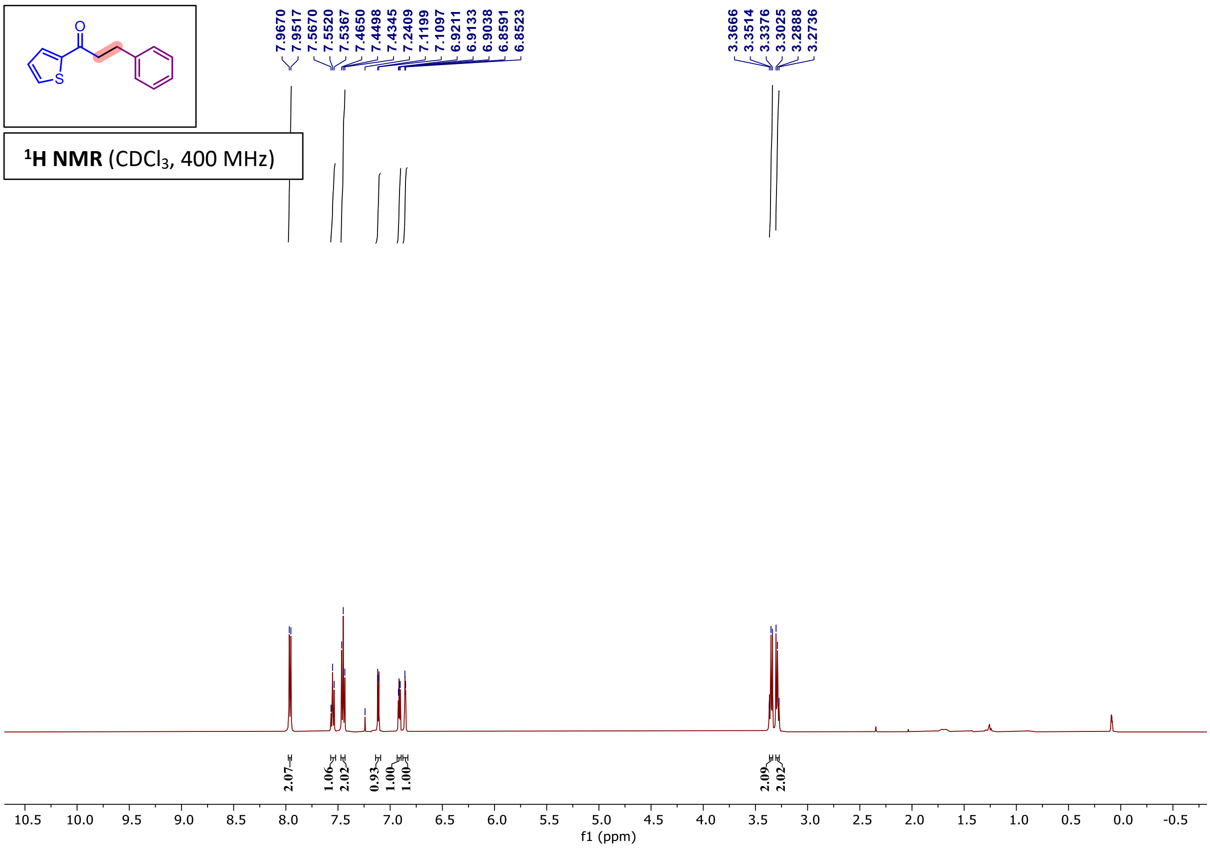

O
13C{1H} NMR (CDCl₃, 100 MHz)
199.25
141.44 135.66 134.26 132.61 129.78 129.62 129.13 128.65 128.55 128.52 127.86 126.85 126.25 123.93
77.42 77.10 76.78
40.65
30.36
f1 (ppm)


8.0502 8.0344 7.9564 7.9526 7.9503 7.9475 7.9400 7.9361 7.8697 7.8531 7.7397 7.7366 7.7276 7.7176 7.7118 7.5352 7.5163 7.5130 7.4753 7.4417 7.4257 7.4107 7.3996 7.3886 7.2410
3.5427 3.5296 3.5128 3.4314 3.4143 3.3995
¹H NMR (CDCl₃, 500 MHz)
H2O
Hexane
1.02 2.00 1.00 1.01 7.01
2.01 2.01
f1 (ppm)

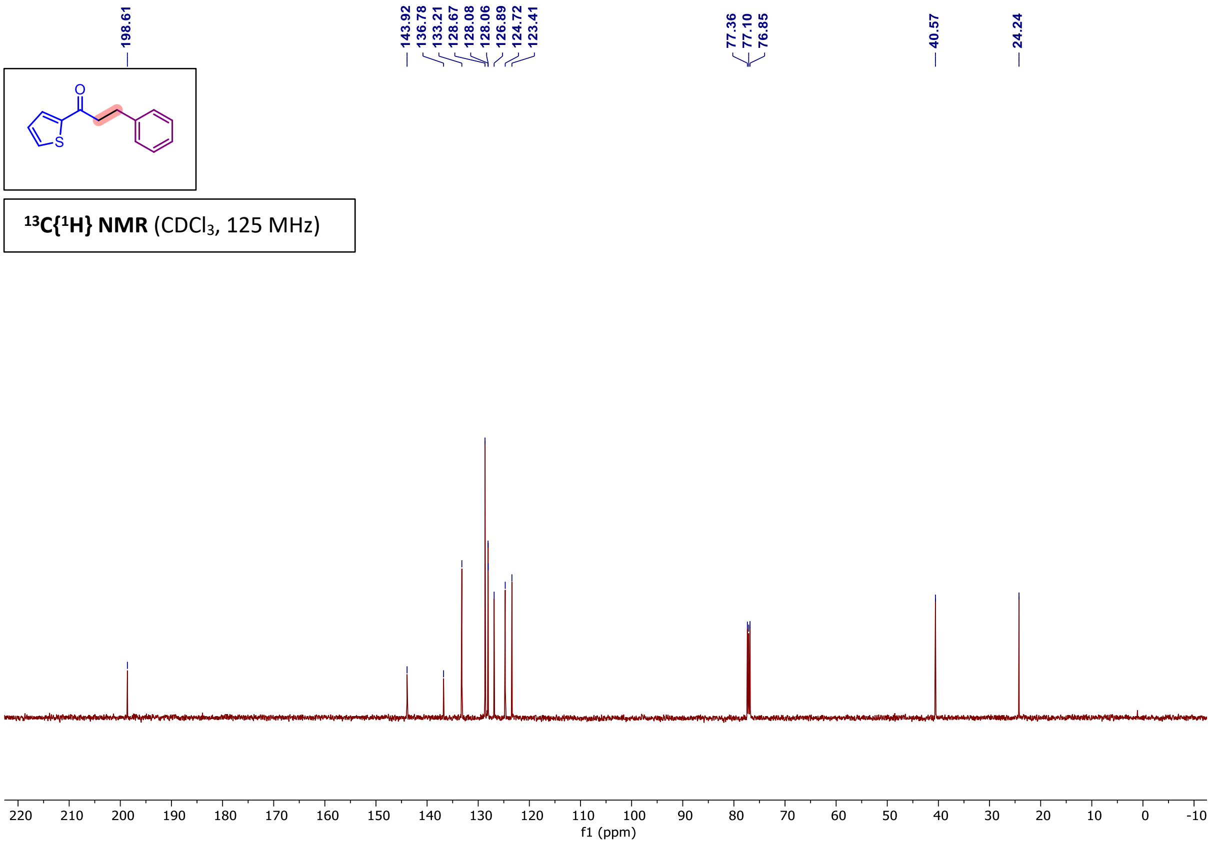

199.42
137.44 136.92 133.20 129.02 128.70 128.14 127.09 126.24 126.18 125.74 125.70 123.60
77.35 77.10 76.84
39.84
27.30
¹³C{¹H} NMR (CDCl₃, 125 MHz)
f1 (ppm)


9.1161 9.1105 8.7270 8.7146 8.7098 8.1830 8.1768 8.1631 8.1574 7.3744 7.3700 7.3623 7.3575 7.3497 7.3385 7.2793 7.2602 7.2419 7.2168 7.1984 7.1857 7.1674
3.2911 3.2726 3.2530 3.0626 3.0435 3.0248
O
N
1H NMR (CDCl3, 400 MHz)
1.00 1.05 1.08 1.08 5.02 2.03 2.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

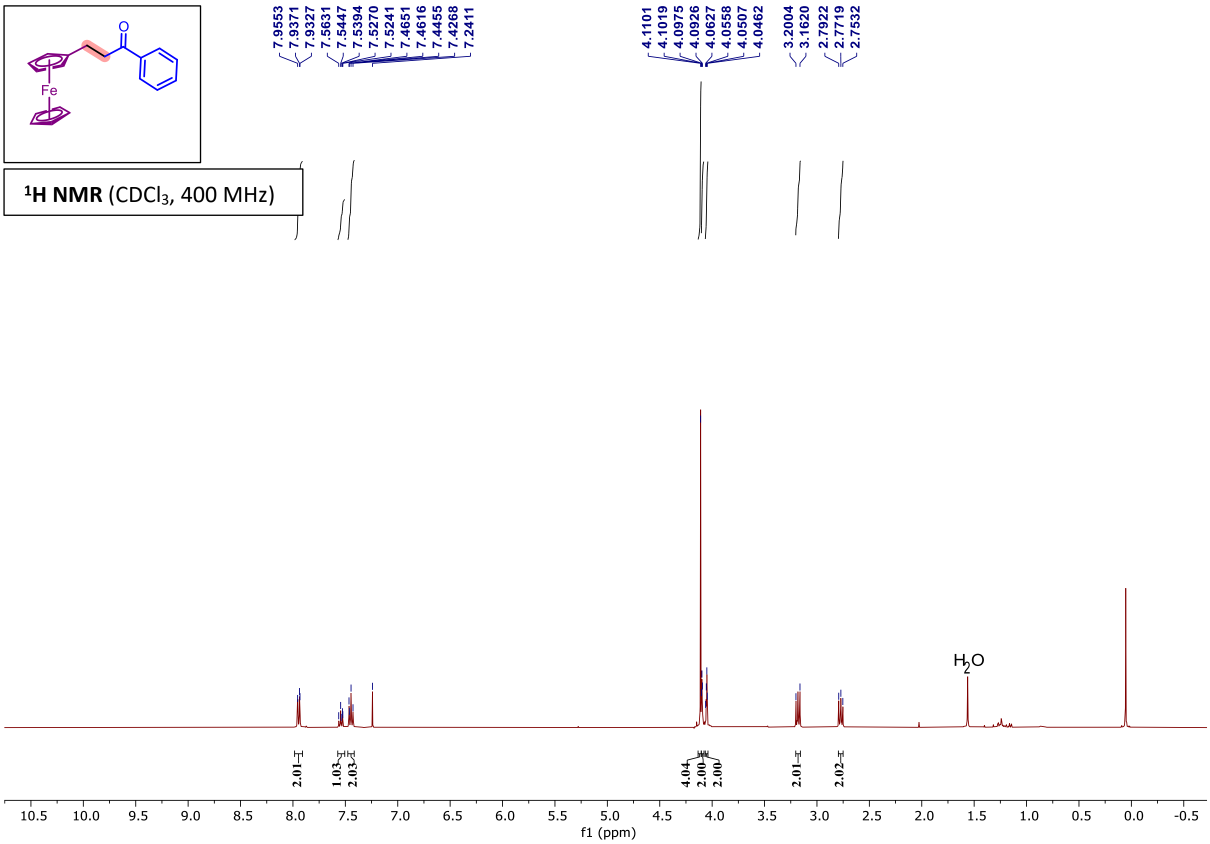

198.02
153.47 149.57
140.75 135.33 132.01 128.59 128.41 126.30 123.64
77.42 77.10 76.78
40.66
29.76
O
N
13C{1H} NMR (CDCl3, 100 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



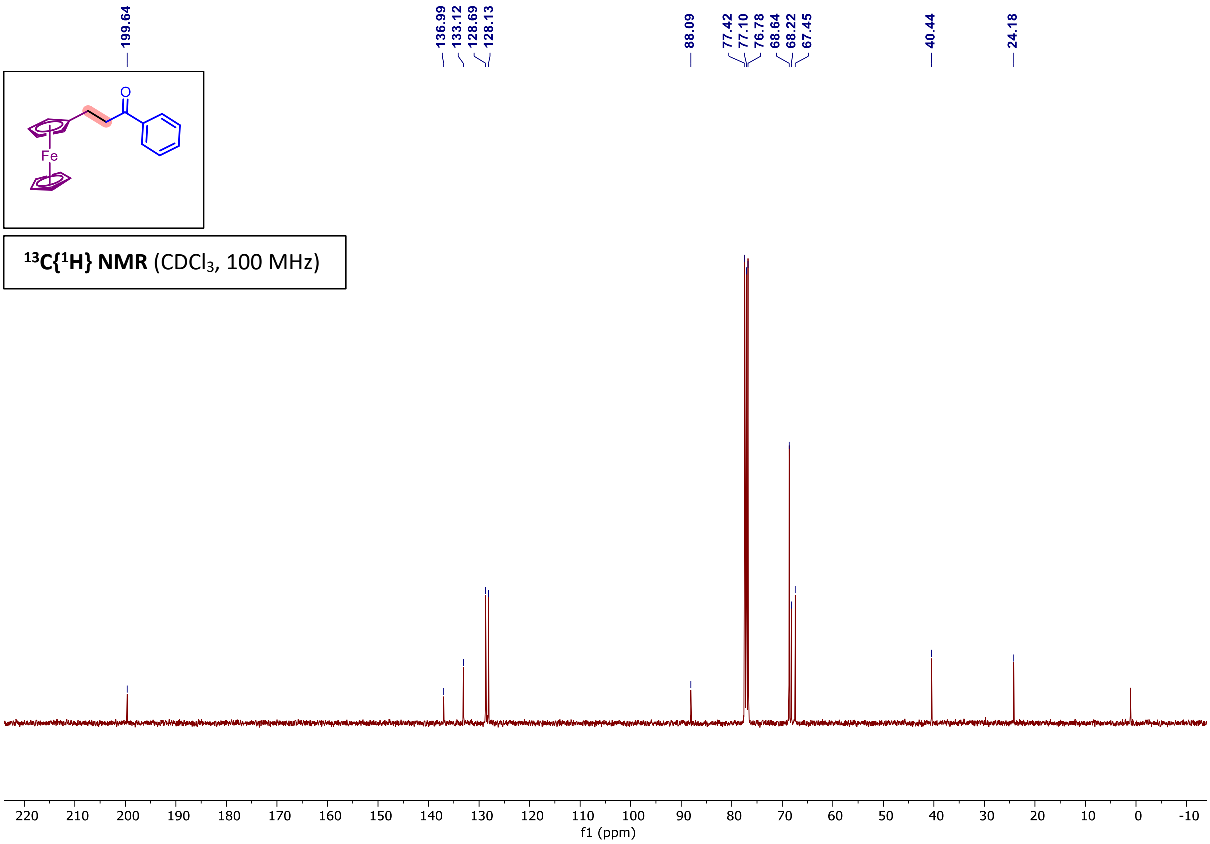
^{1}H NMR ($CDCl_3$, 400 MHz)



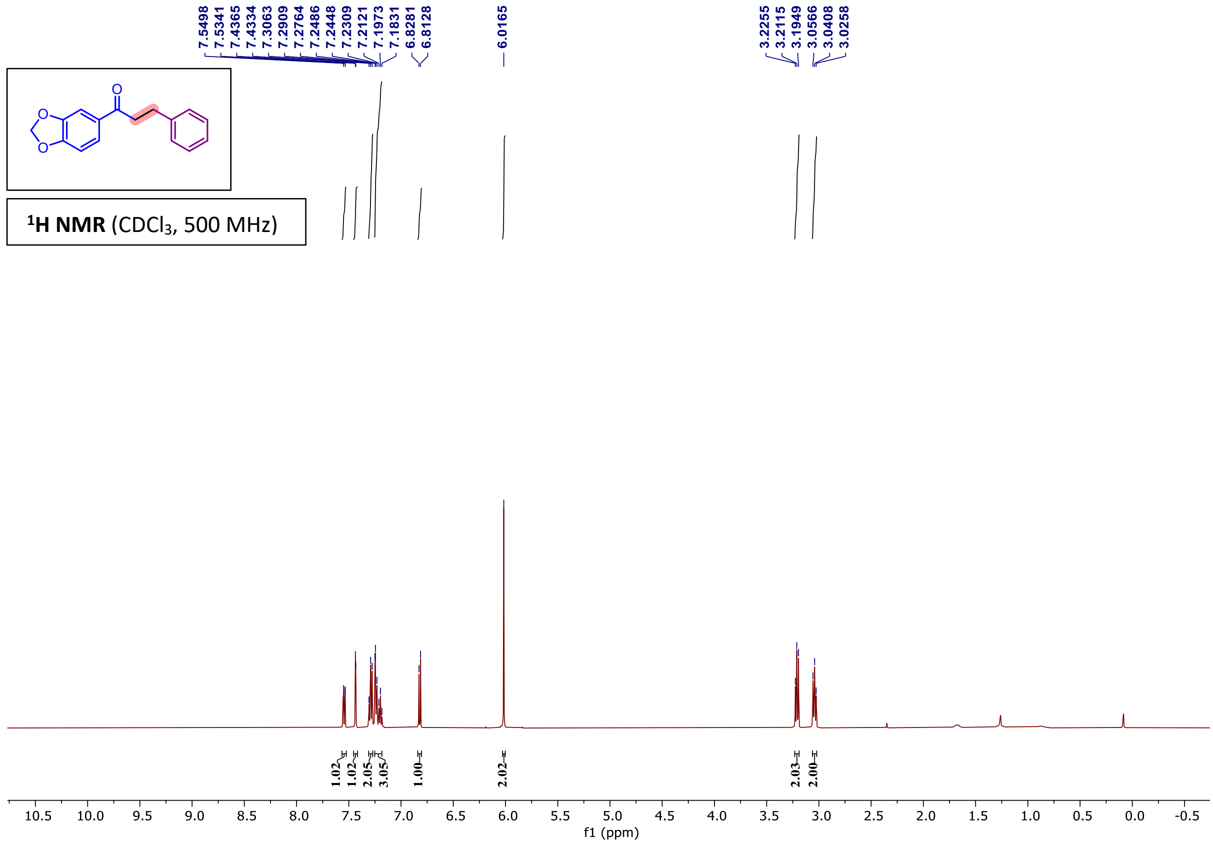
^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)



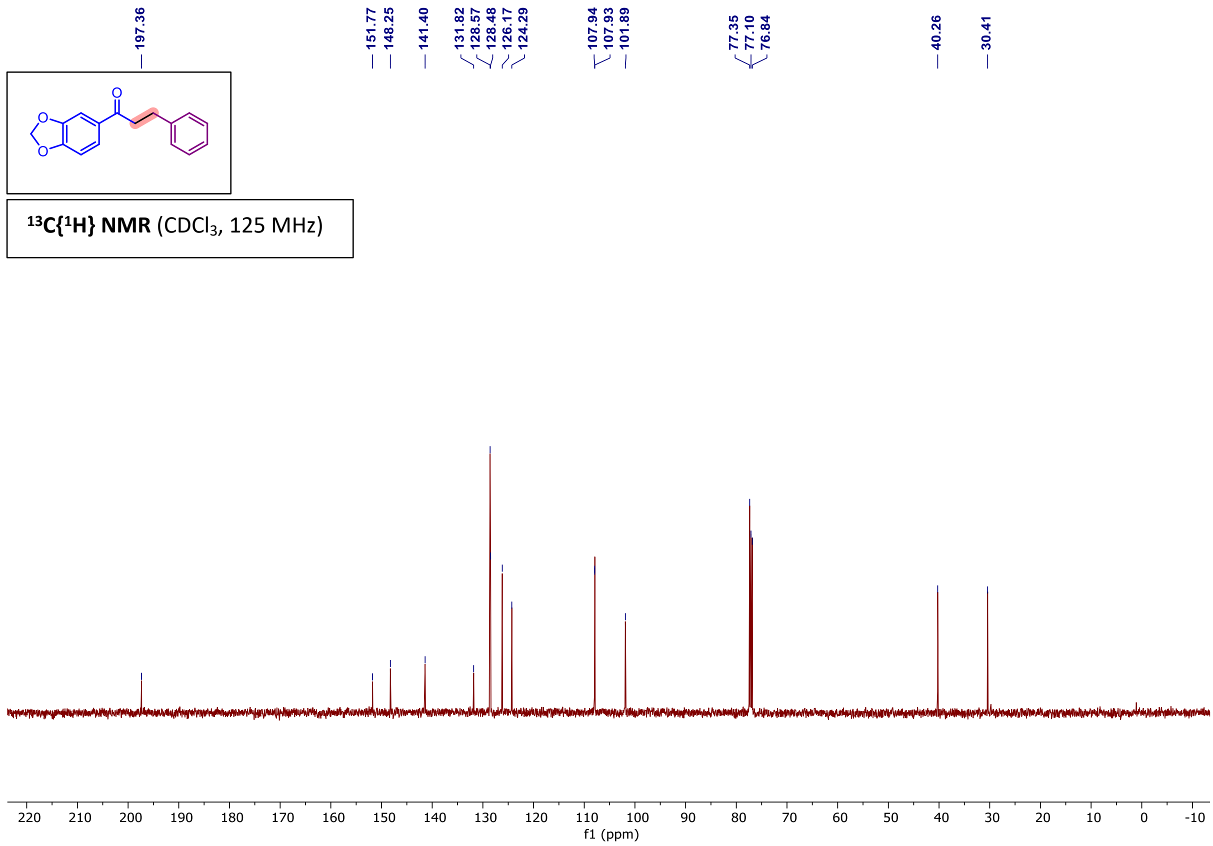
^{1}H NMR ($CDCl_3$, 400 MHz)



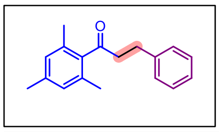
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)



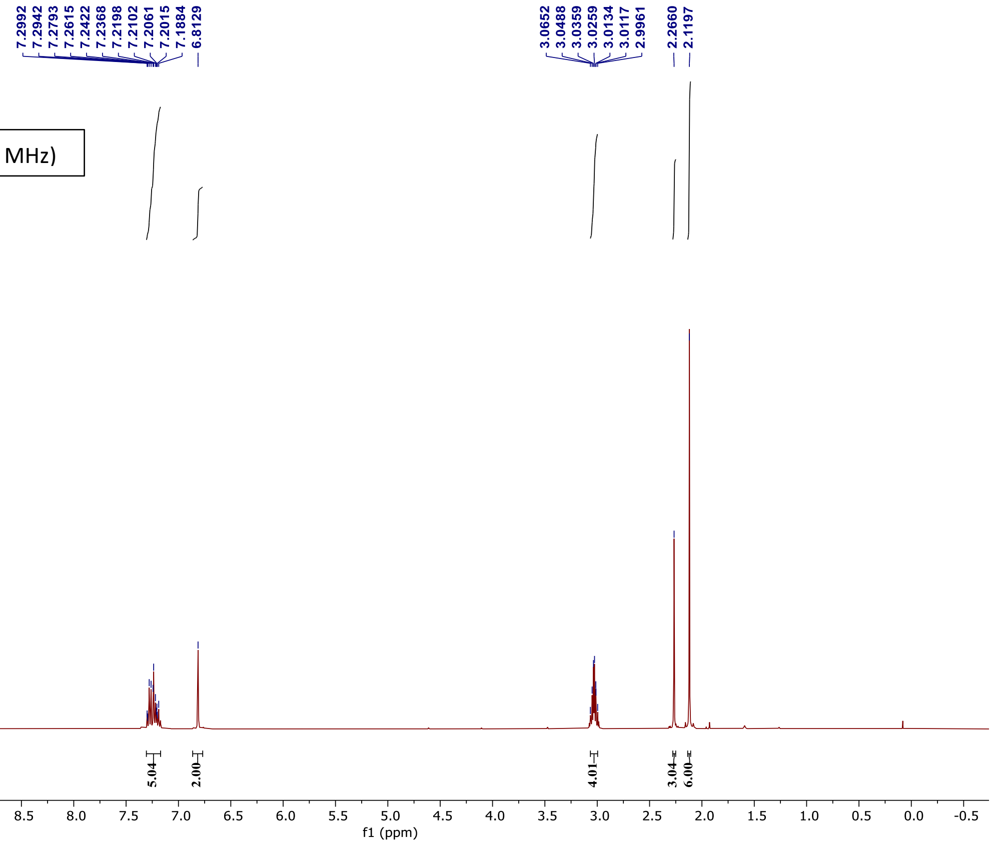
7.5498
7.5341
7.4365
7.4334
7.3063
7.2909
7.2764
7.2486
7.2448
7.2309
7.2121
7.1973
7.1831
6.8281
6.8128
6.0165
3.2255
3.2115
3.1949
3.0566
3.0408
3.0258
1H NMR (CDCl3, 500 MHz)
1.02
1.02
2.05
3.05
1.00
2.02
2.03
2.00
f1 (ppm)

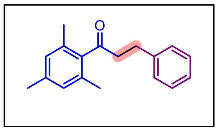


197.36
151.77
148.25
141.40
131.82
128.57
128.48
126.17
124.29
107.94
107.93
101.89
77.35
77.10
76.84
40.26
30.41
13C{1H} NMR (CDCl3, 125 MHz)
f1 (ppm)

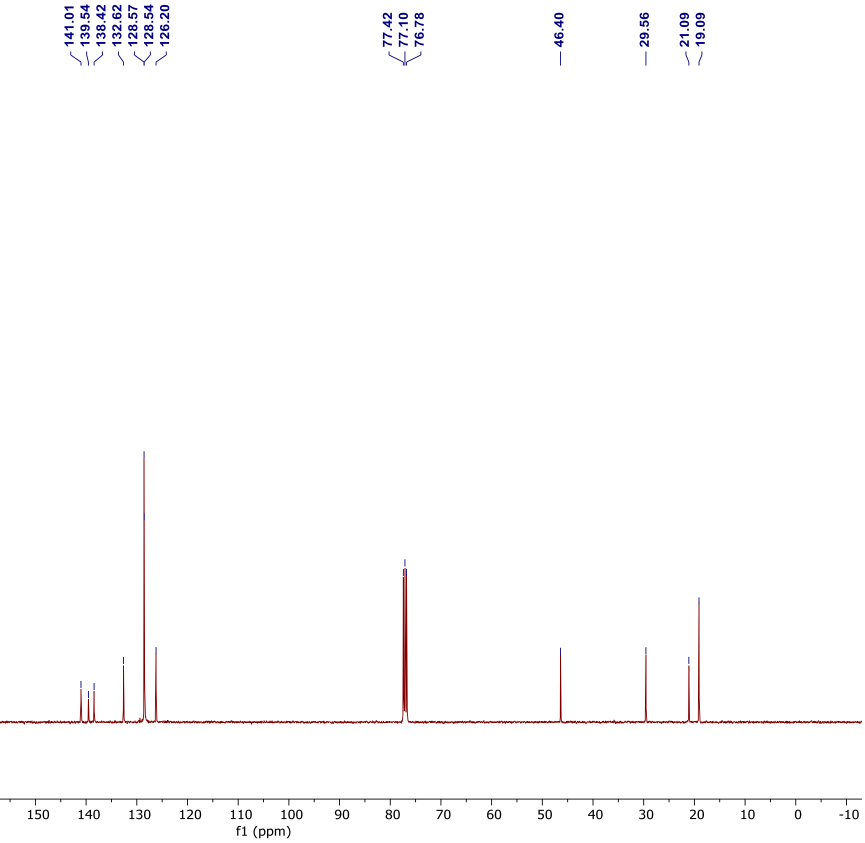


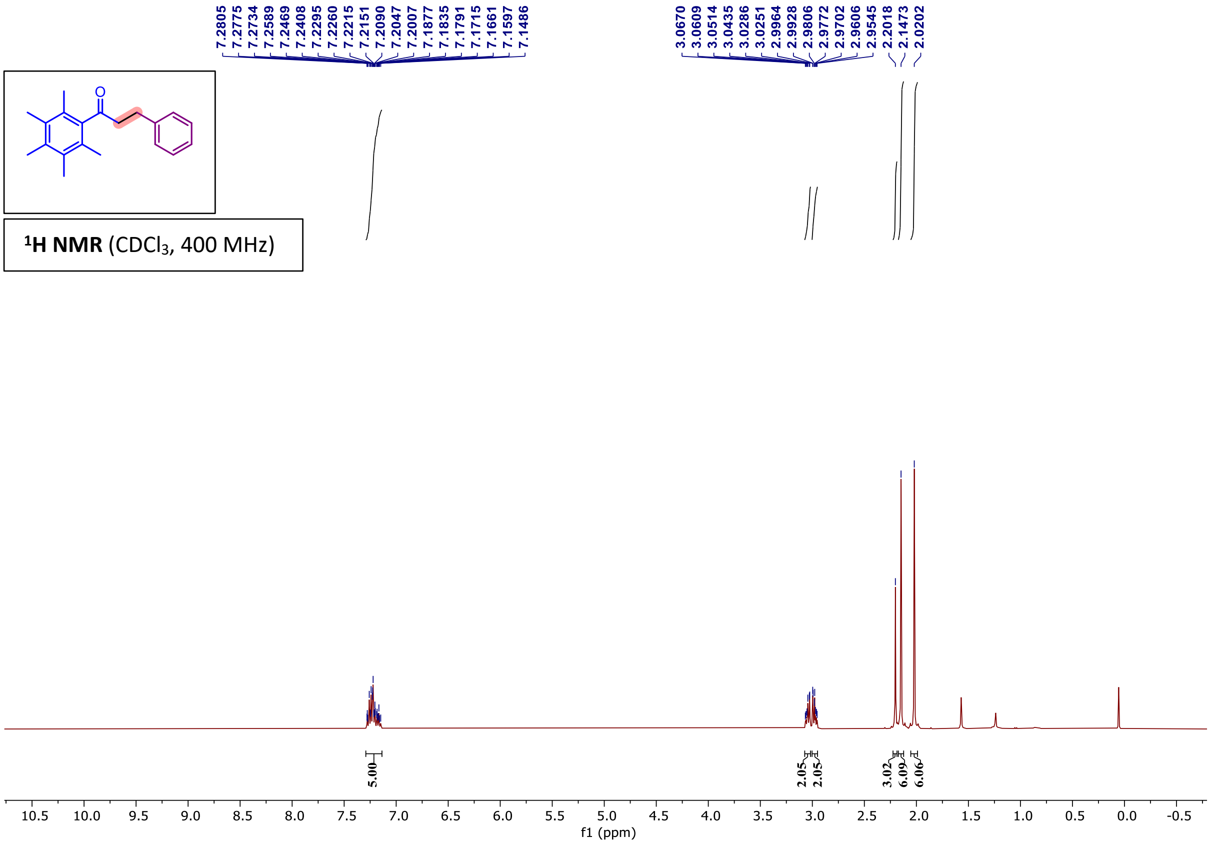
^{1}H NMR ($CDCl_3$, 400 MHz)



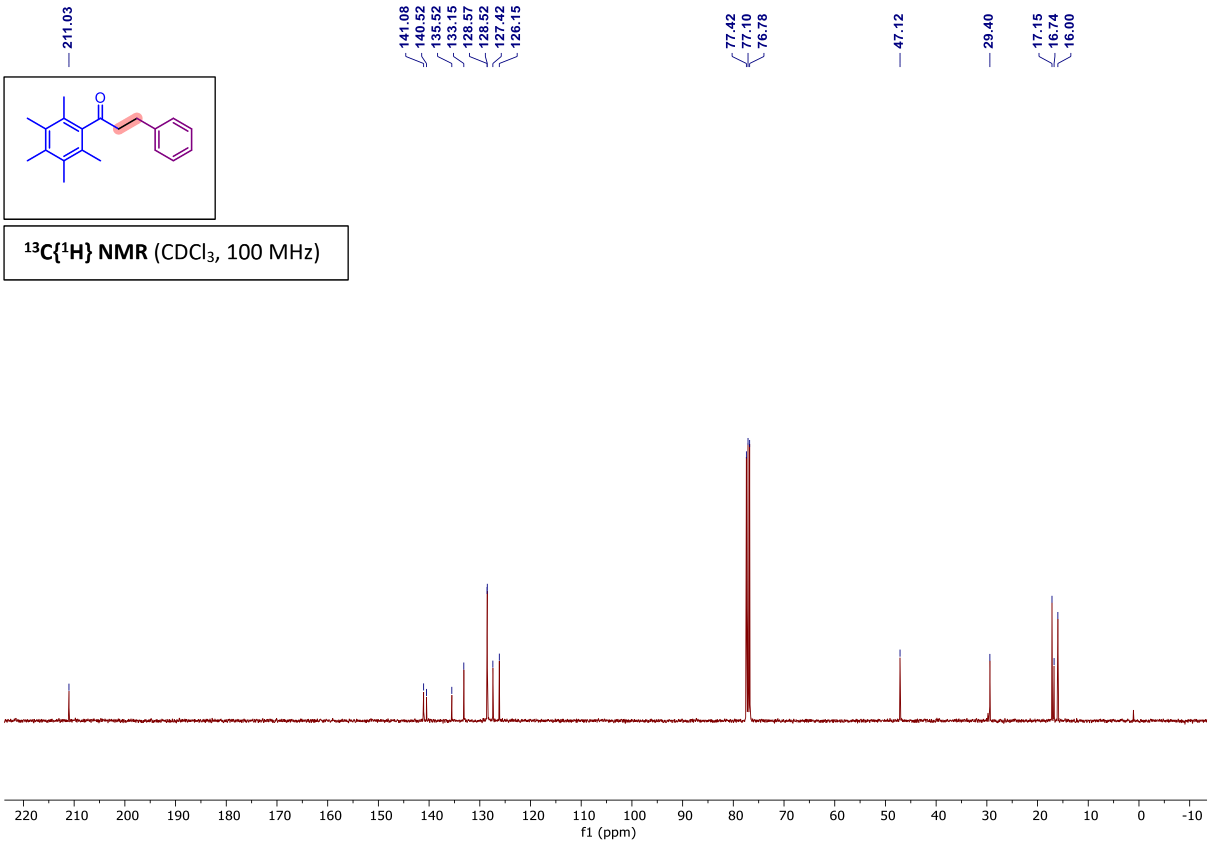


^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)

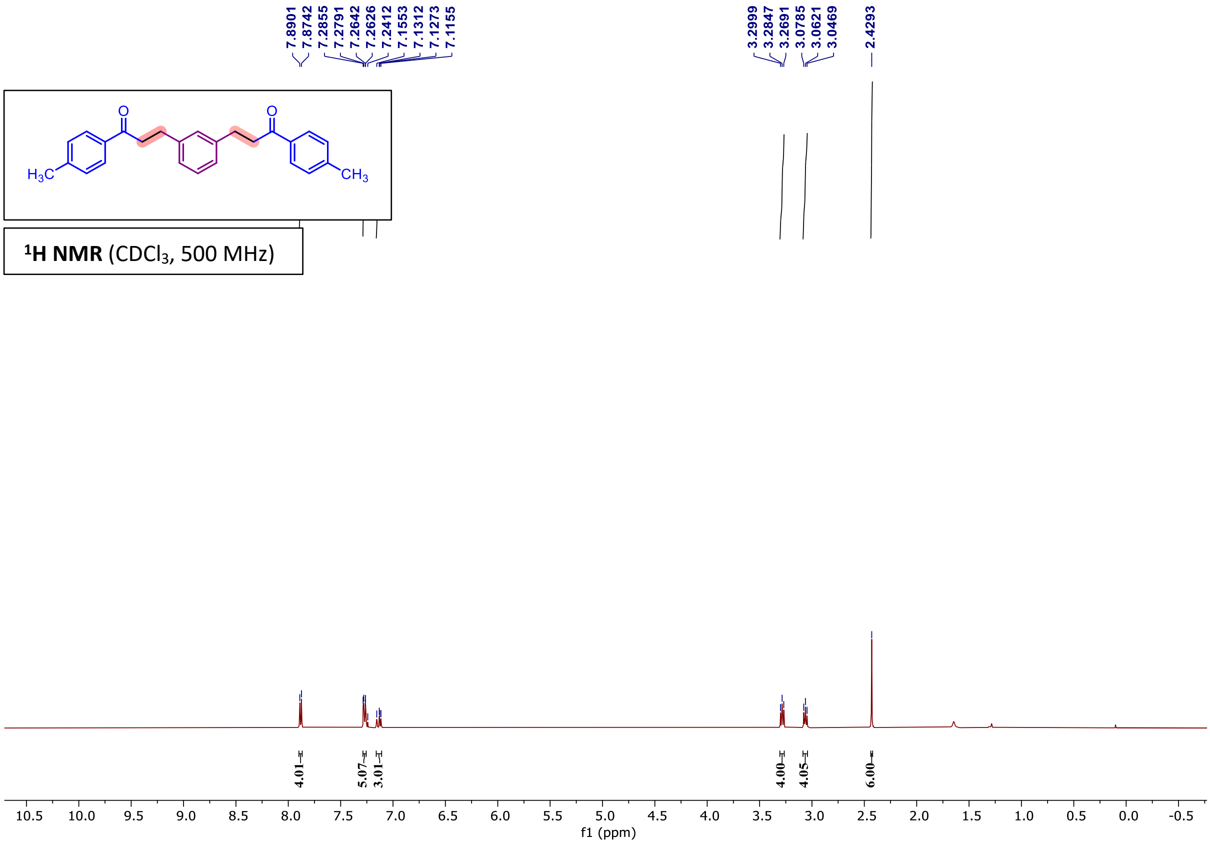


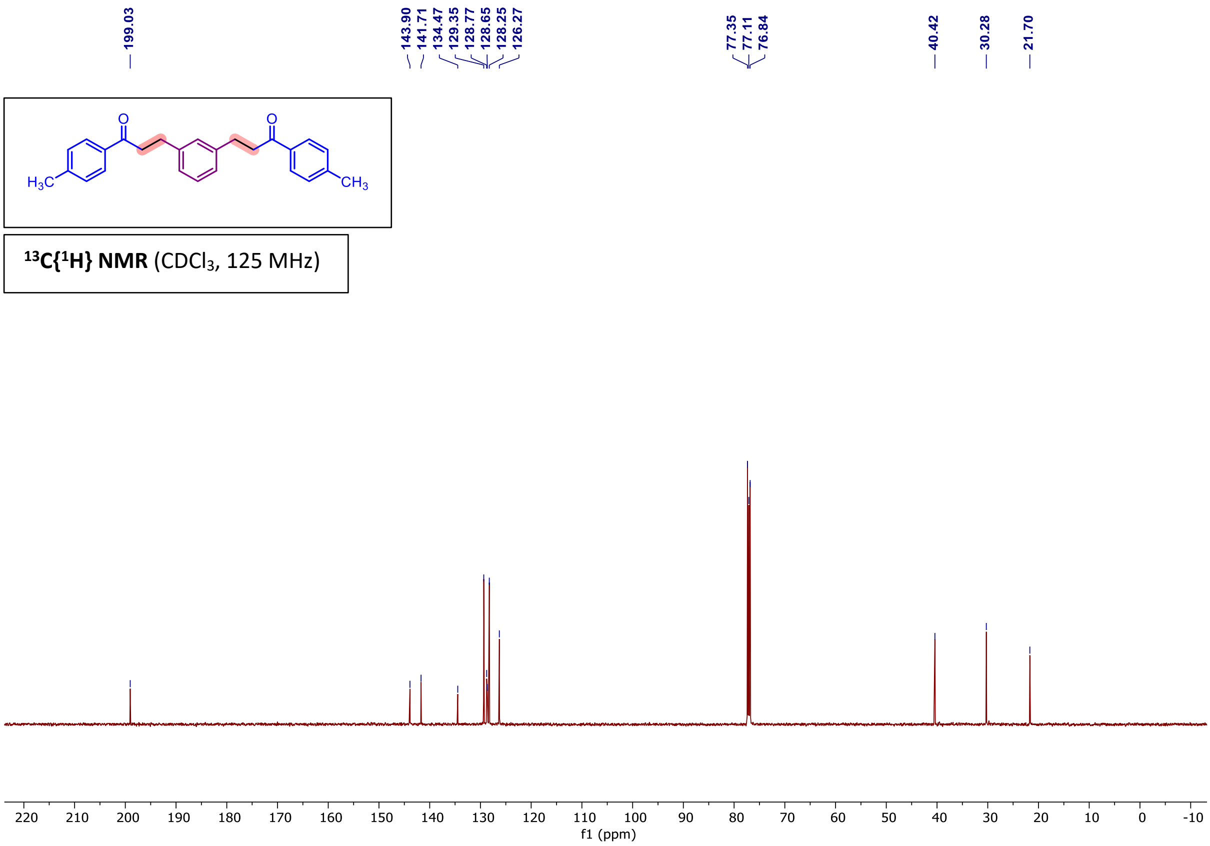


O
^{1}H NMR (CDCl$_3$, 400 MHz)
7.2805 7.2775 7.2734 7.2589 7.2469 7.2408 7.2295 7.2260 7.2215 7.2151 7.2090 7.2047 7.2007 7.1877 7.1835 7.1791 7.1715 7.1661 7.1597 7.1486
3.0670 3.0609 3.0514 3.0435 3.0286 3.0251 2.9964 2.9928 2.9806 2.9772 2.9702 2.9606 2.9545 2.2018 2.1473 2.0202
5.00
2.05 2.05
3.02 6.09 6.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

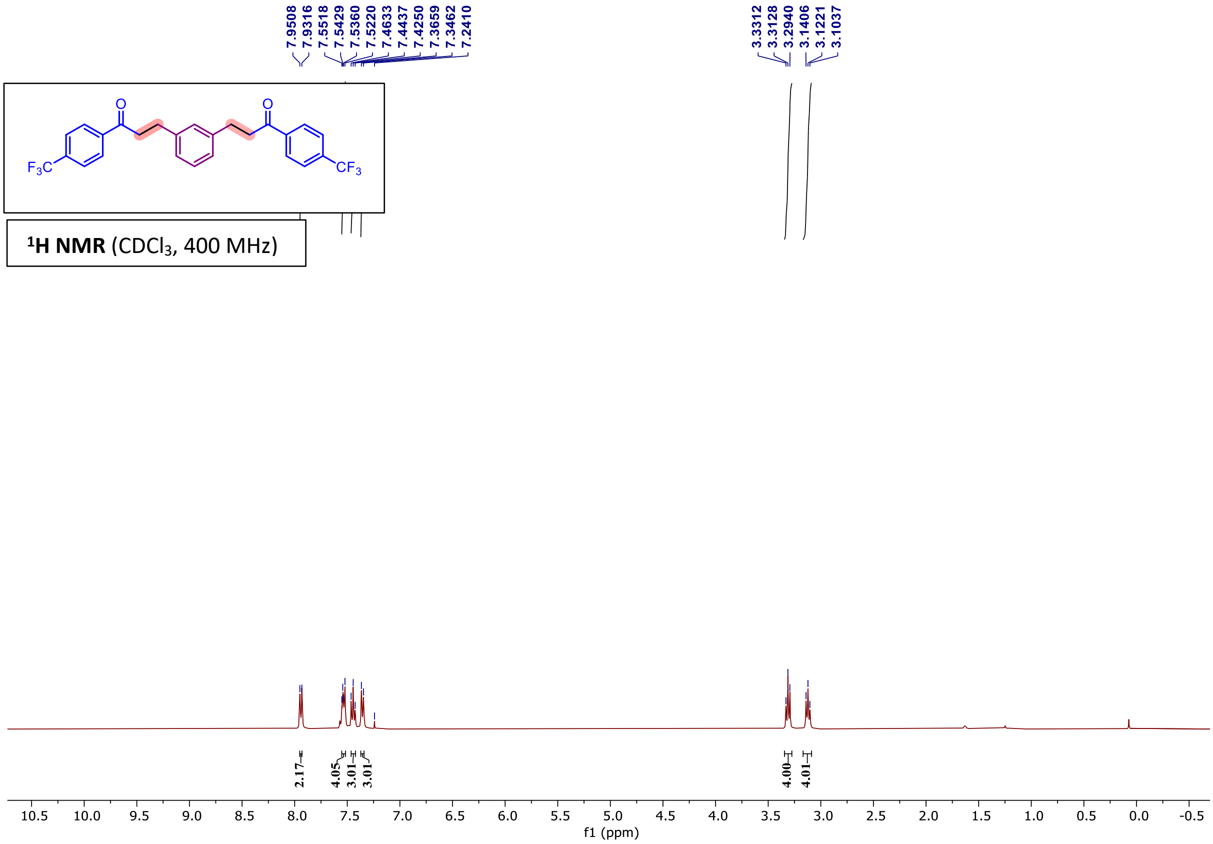


211.03
141.08 140.52 135.52 133.15 128.57 128.52 127.42 126.15
77.42 77.10 76.78
47.12
29.40
17.15 16.74 16.00
O
^{13}C{^{1}H} NMR (CDCl$_3$, 100 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

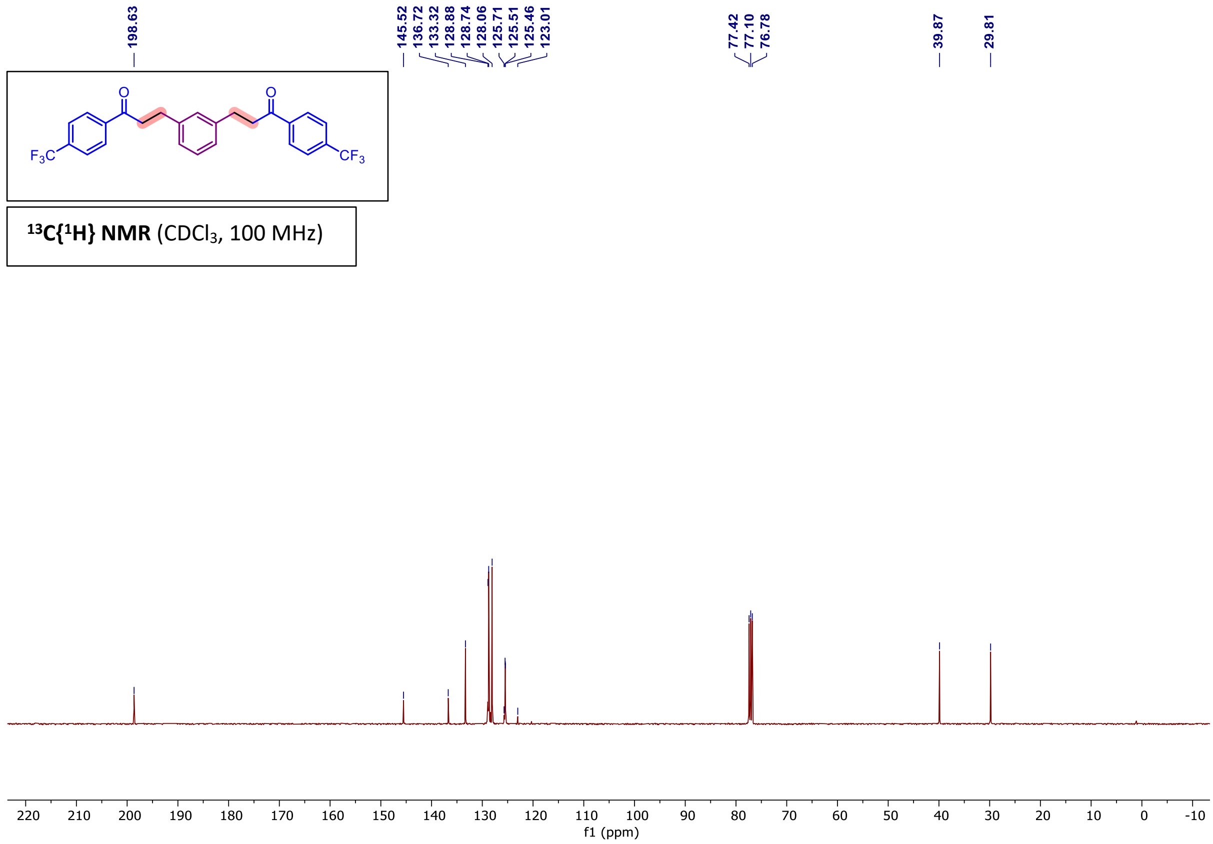

7.8901
7.8742
7.2855
7.2791
7.2642
7.2626
7.2412
7.1553
7.1312
7.1273
7.1155
3.2999
3.2847
3.2691
3.0785
3.0621
3.0469
2.4293
H3C
CH3
O
O
1H NMR (CDCl3, 500 MHz)
4.01
5.07
3.01
4.00
4.05
6.00
f1 (ppm)

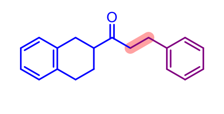

199.03
143.90
141.71
134.47
129.35
128.77
128.65
128.25
126.27
77.35
77.11
76.84
40.42
30.28
21.70
H3C
CH3
O
O
13C{1H} NMR (CDCl3, 125 MHz)
f1 (ppm)

¹H NMR (CDCl$_3$, 400 MHz)

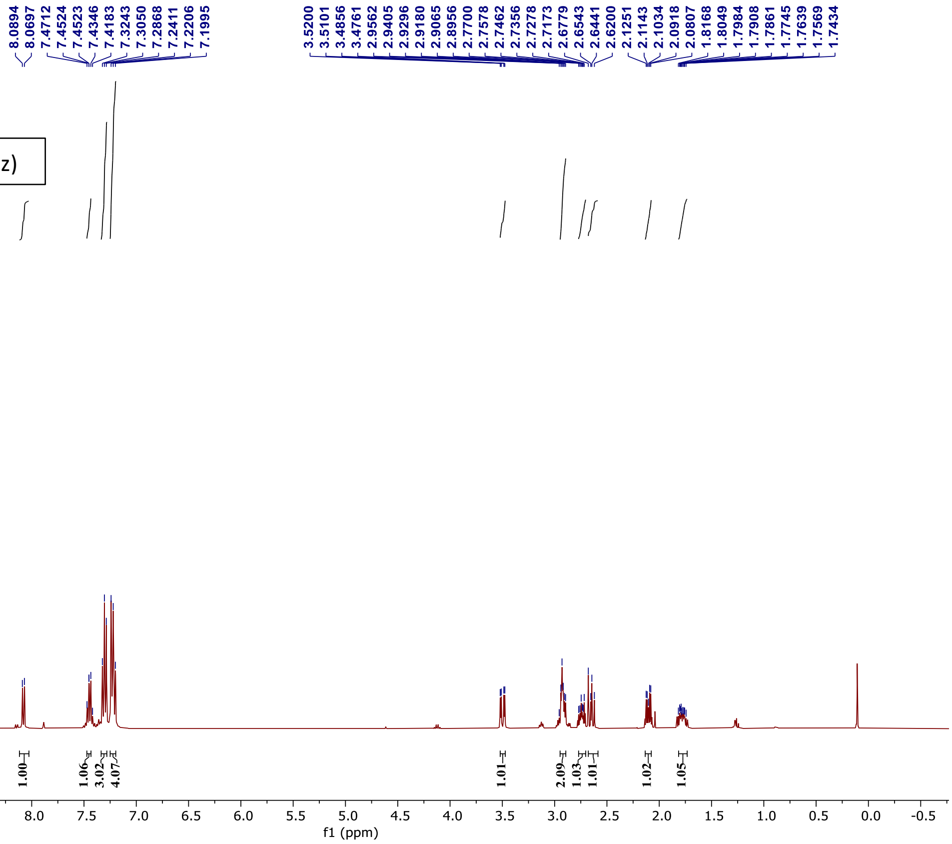


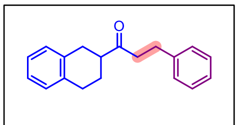
¹³C{¹H} NMR (CDCl$_3$, 100 MHz)



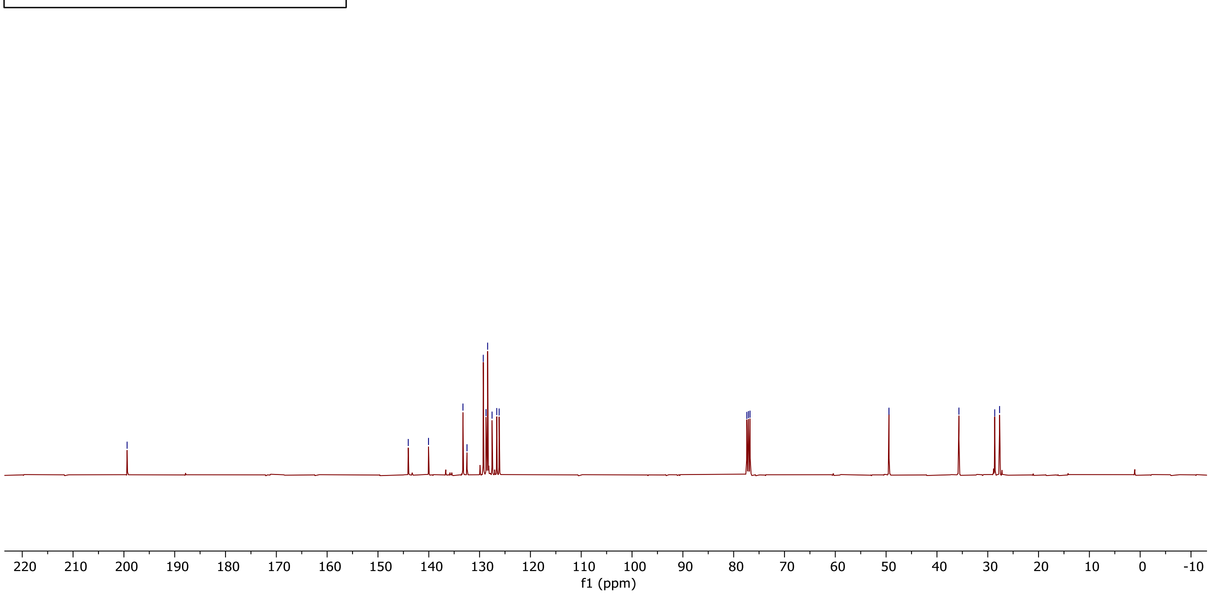


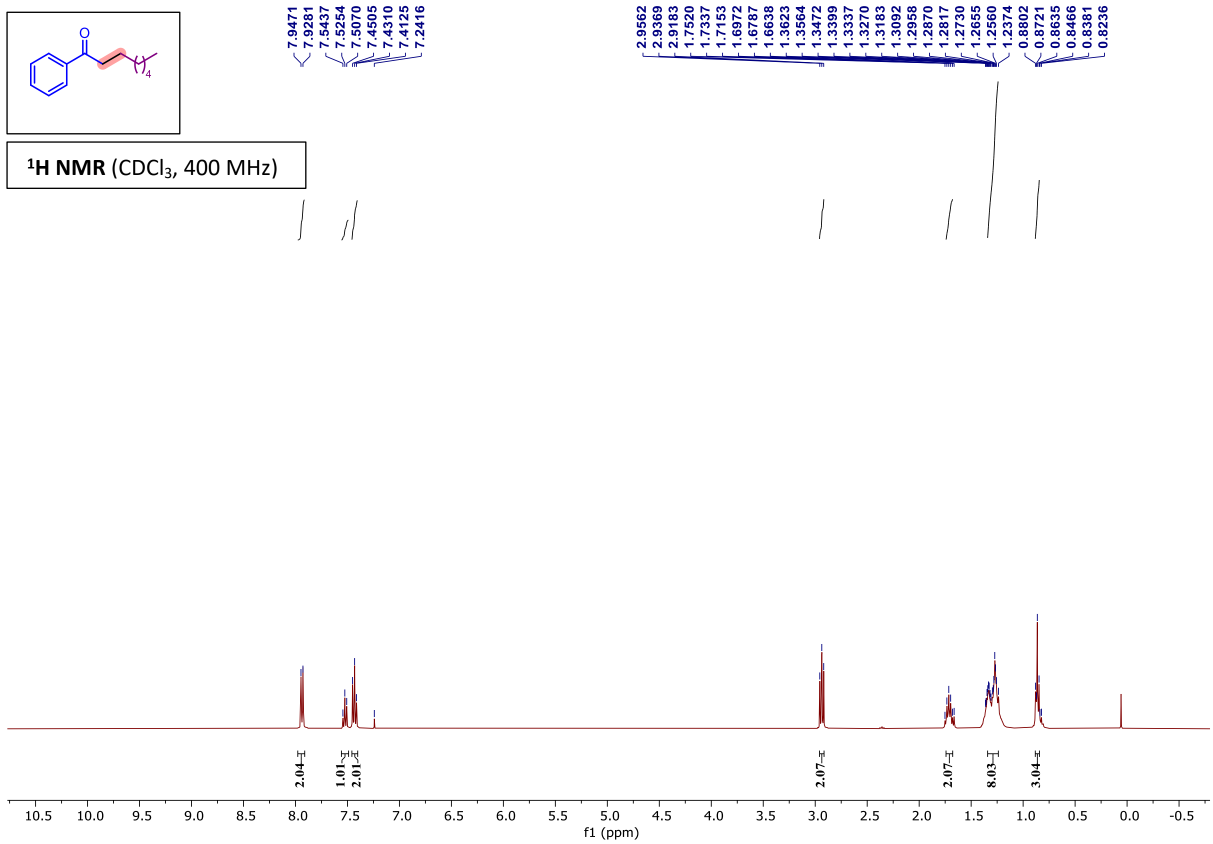
¹H NMR ($CDCl_3$, 400 MHz)



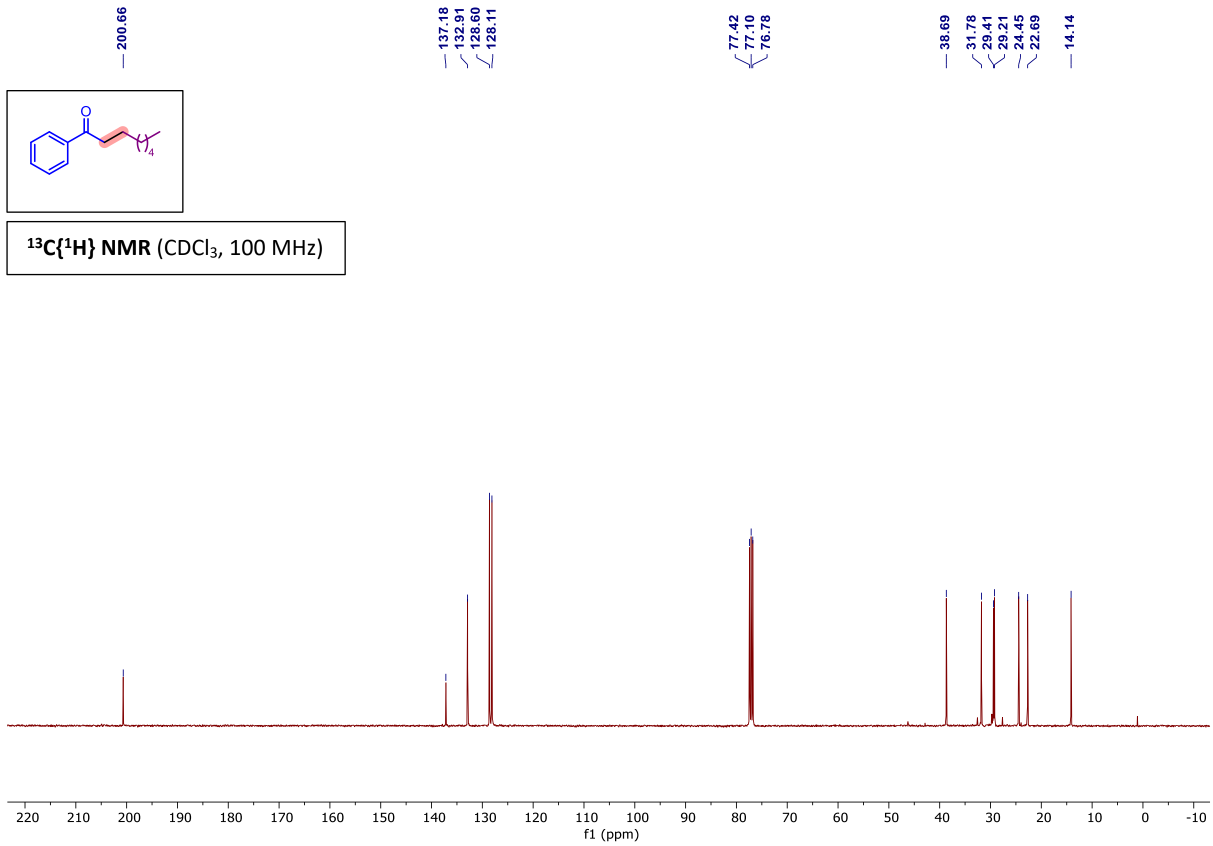


¹³C{¹H} NMR ($CDCl_3$, 100 MHz)

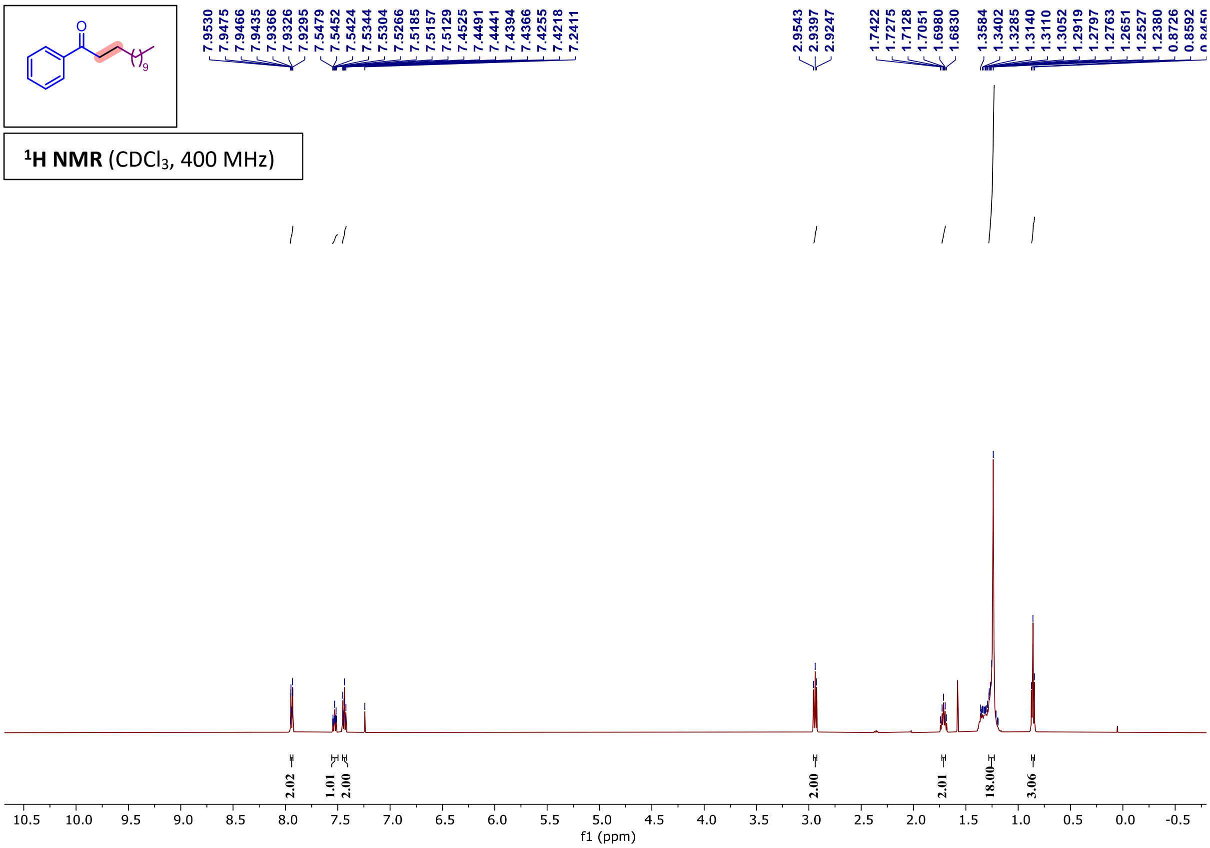


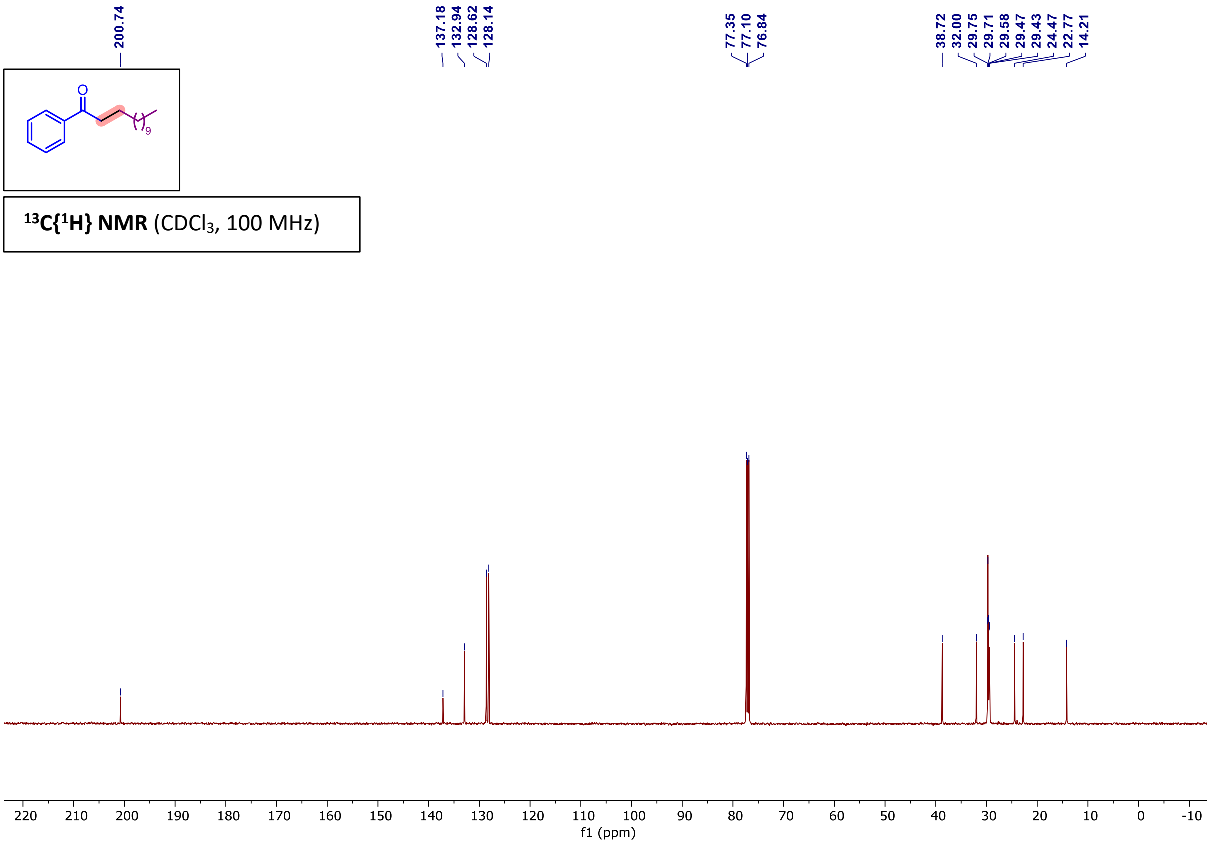


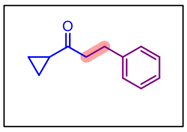
^{1}H NMR ($CDCl_3$, 400 MHz)



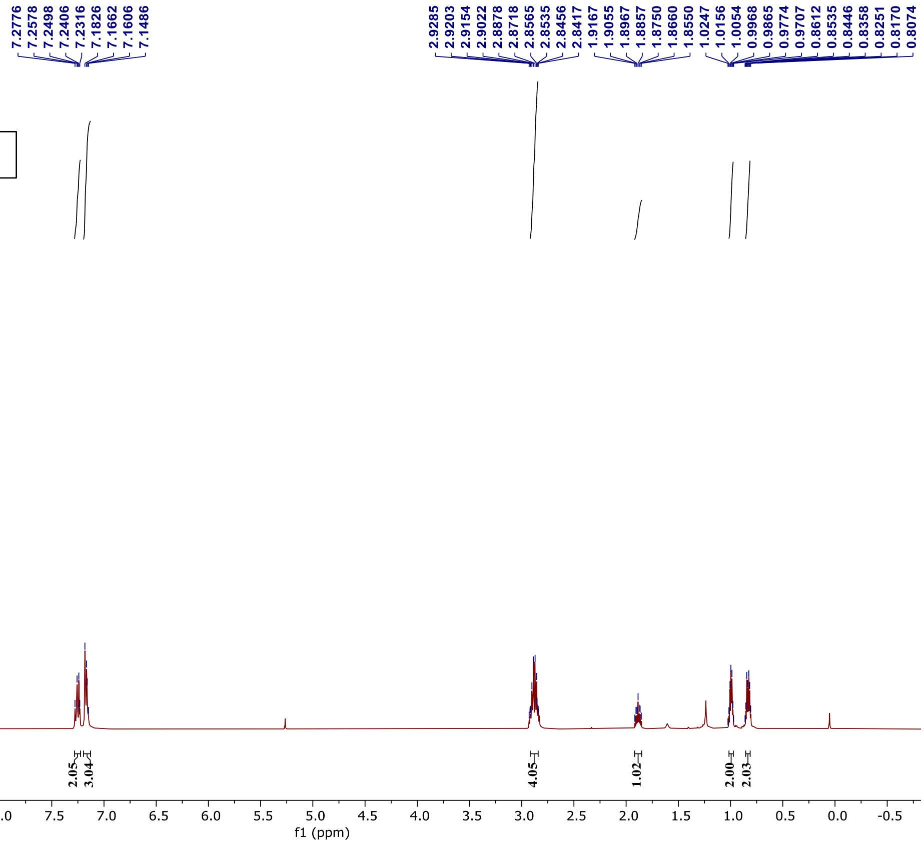
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)

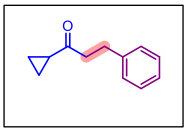

O
9
¹H NMR (CDCl3, 400 MHz)
7.9530 7.9475 7.9466 7.9435 7.9366 7.9326 7.9295 7.5479 7.5452 7.5424 7.5344 7.5304 7.5266 7.5185 7.5157 7.5129 7.4525 7.4491 7.4441 7.4394 7.4366 7.4255 7.4218 7.2411
2.9543 2.9397 2.9247
1.7422 1.7275 1.7128 1.7051 1.6980 1.6830
1.3584 1.3402 1.3285 1.3140 1.3110 1.3052 1.2919 1.2797 1.2763 1.2651 1.2527 1.2380 0.8726 0.8592
2.02 1.01 2.00 2.00 2.01 18.00 3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


200.74
137.18 132.94 128.62 128.14
77.35 77.10 76.84
38.72 32.00 29.75 29.71 29.58 29.47 29.43 24.47 22.77 14.21
O
9
¹³C{¹H} NMR (CDCl3, 100 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

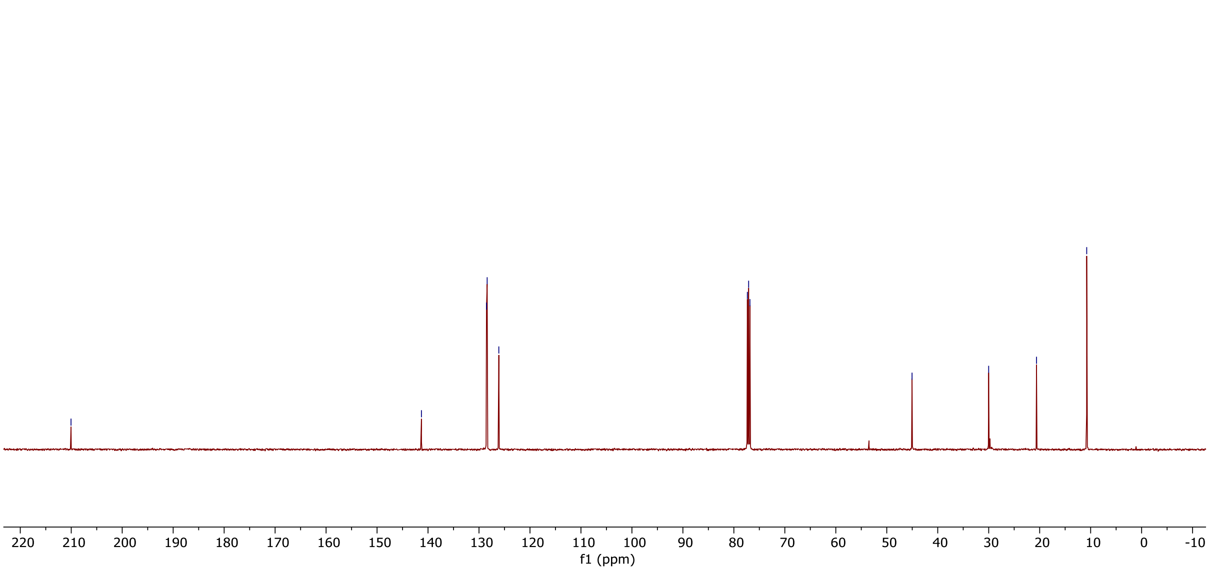


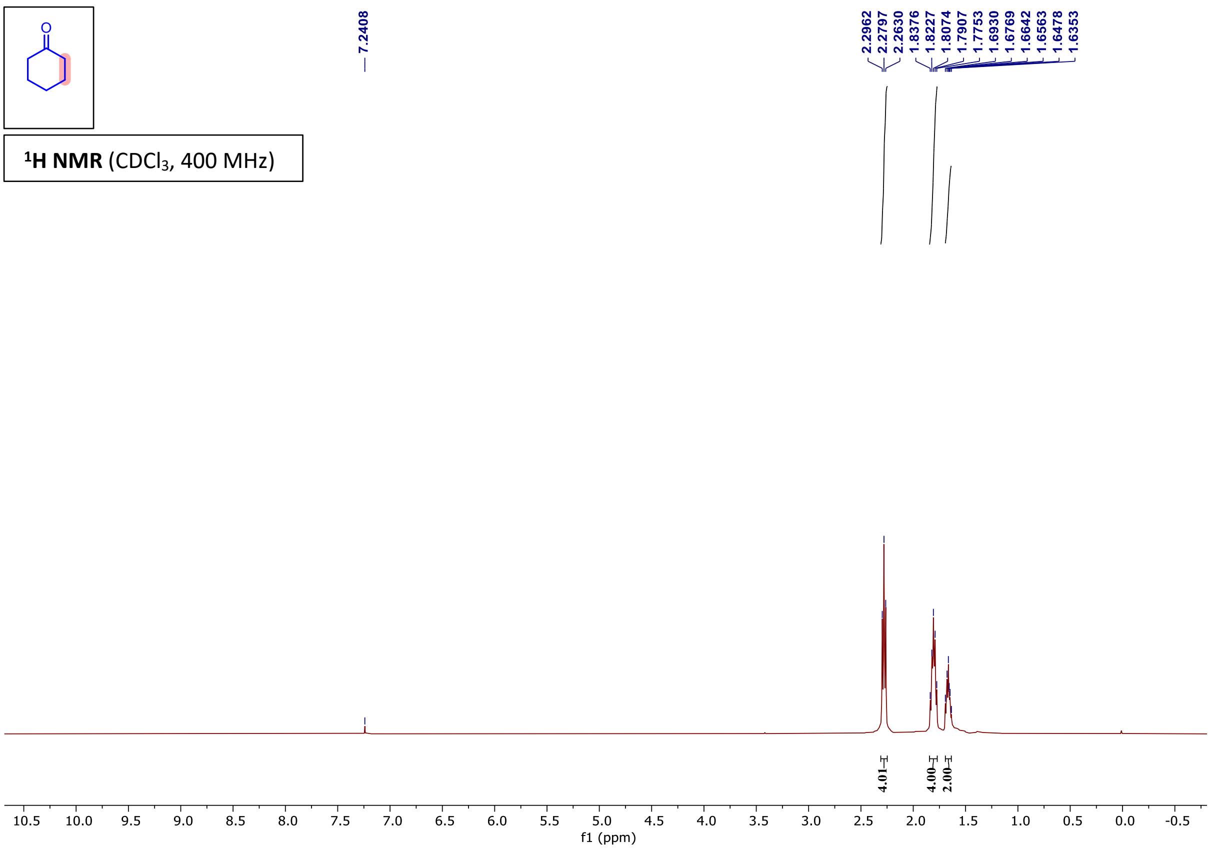
¹H NMR ($CDCl_3$, 400 MHz)



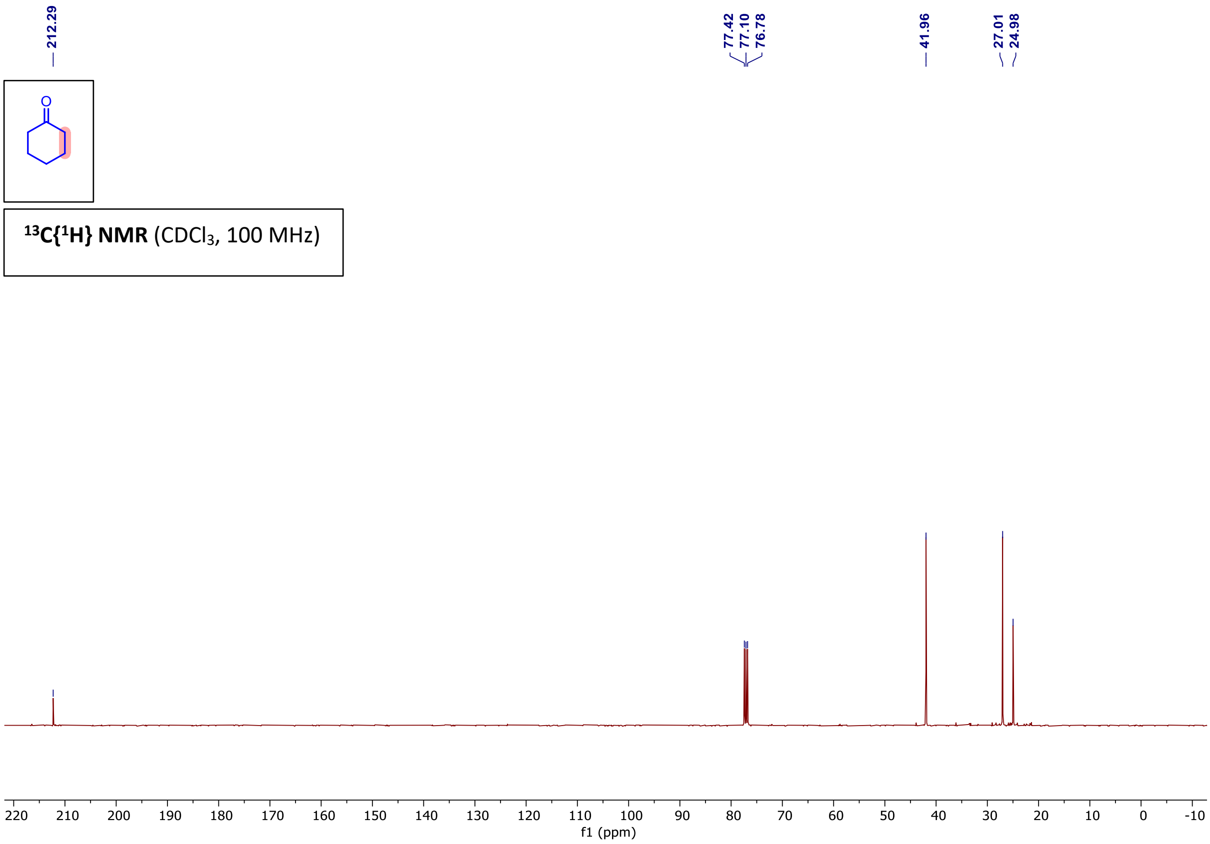


¹³C{¹H} NMR ($CDCl_3$, 125 MHz)

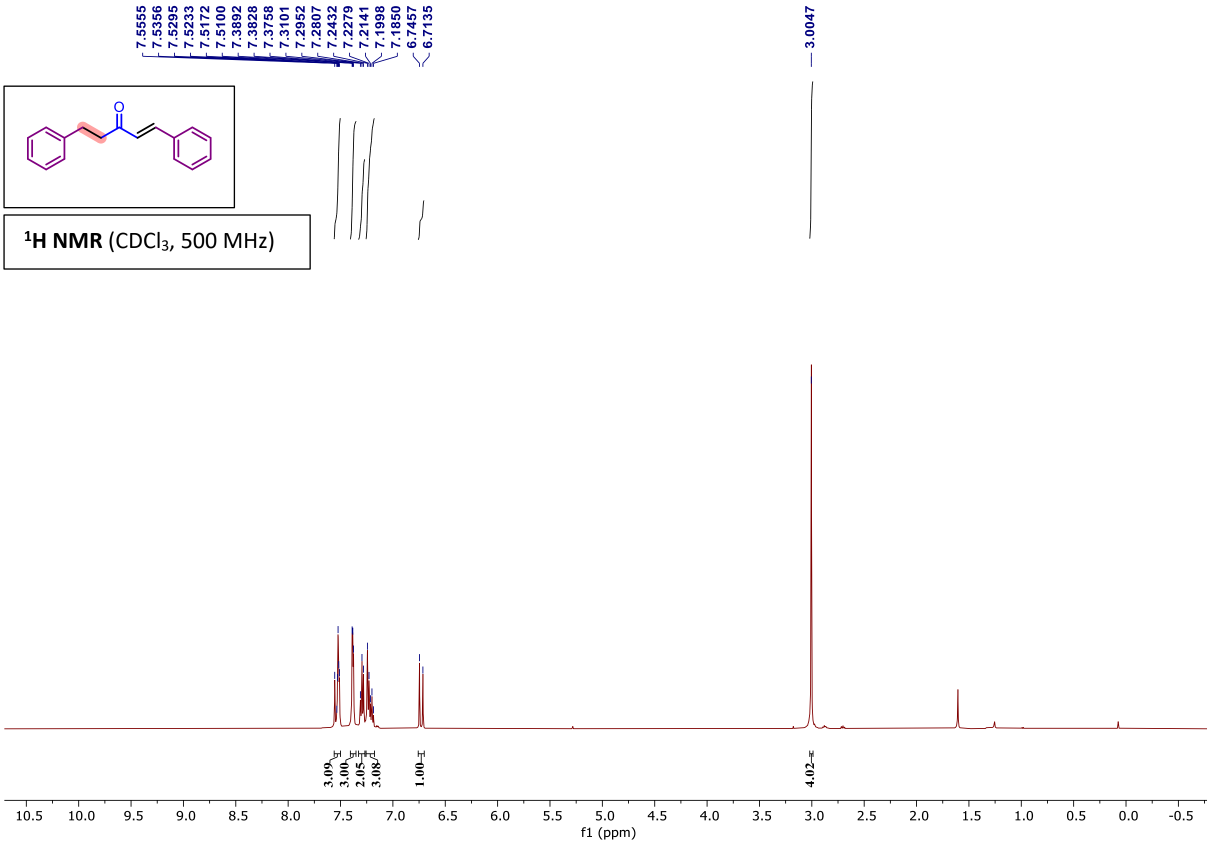




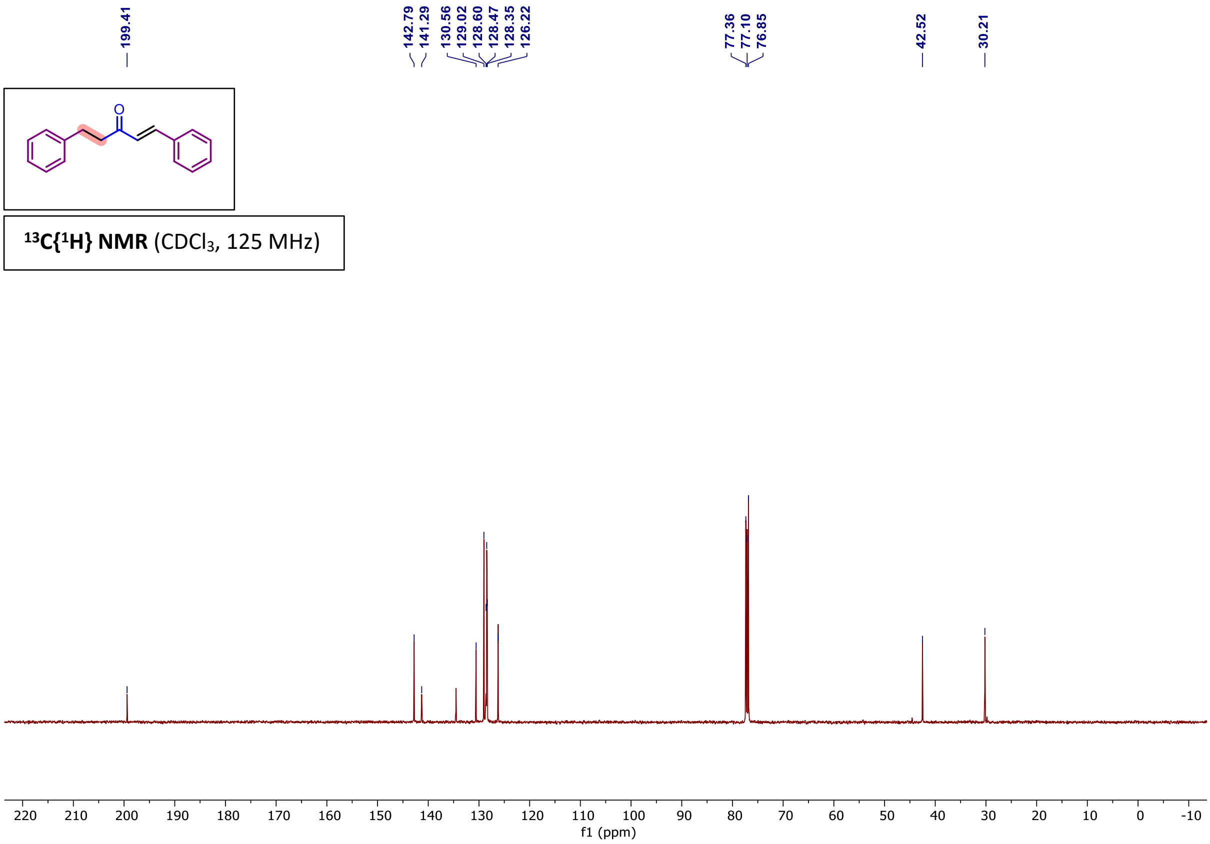
^{1}H NMR (CDCl$_3$, 400 MHz)



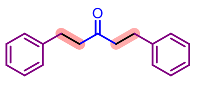
^{13}C{^{1}H} NMR (CDCl$_3$, 100 MHz)



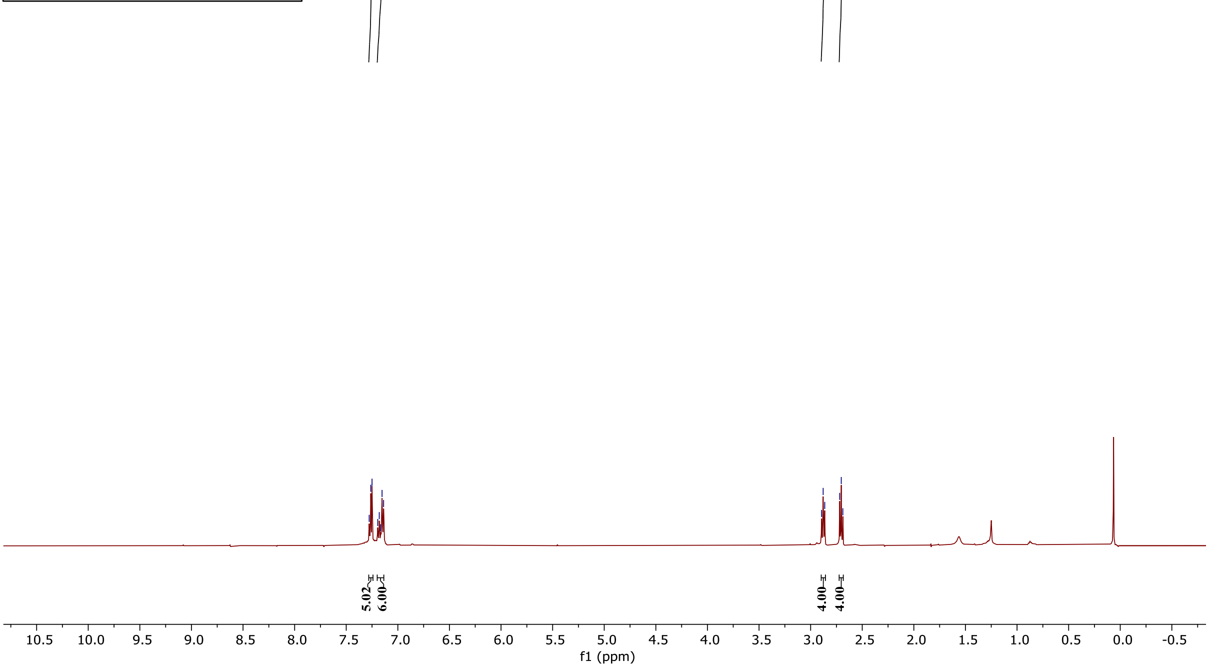
^{1}H NMR ($CDCl_3$, 500 MHz)

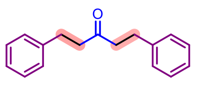


^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)

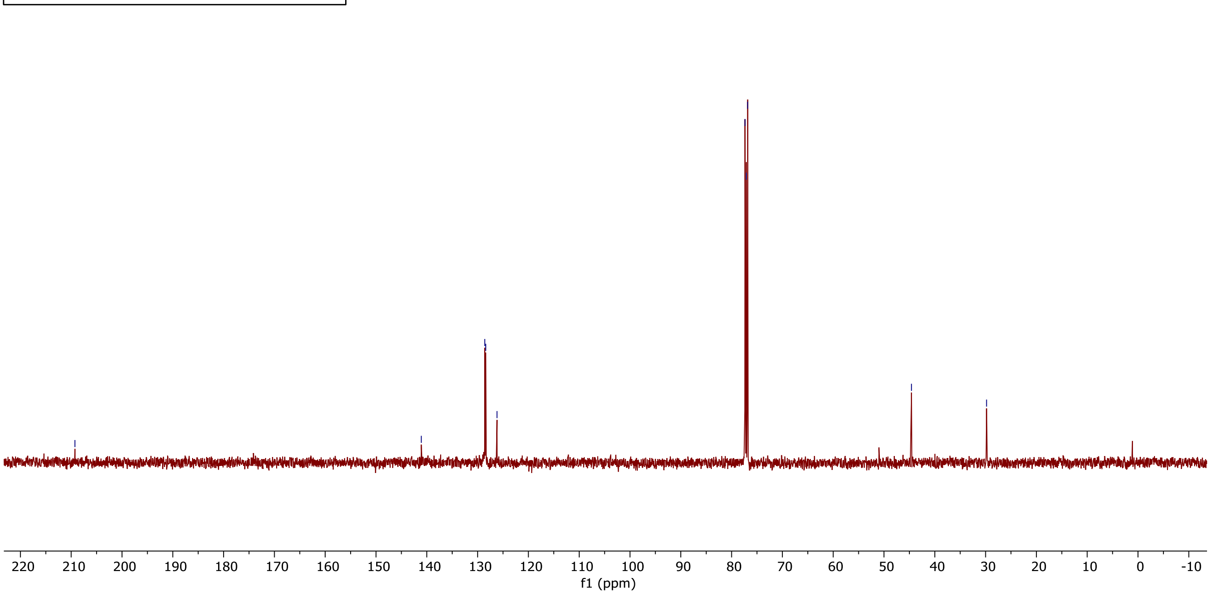


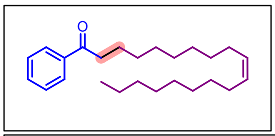
^{1}H NMR ($CDCl_3$, 500 MHz)



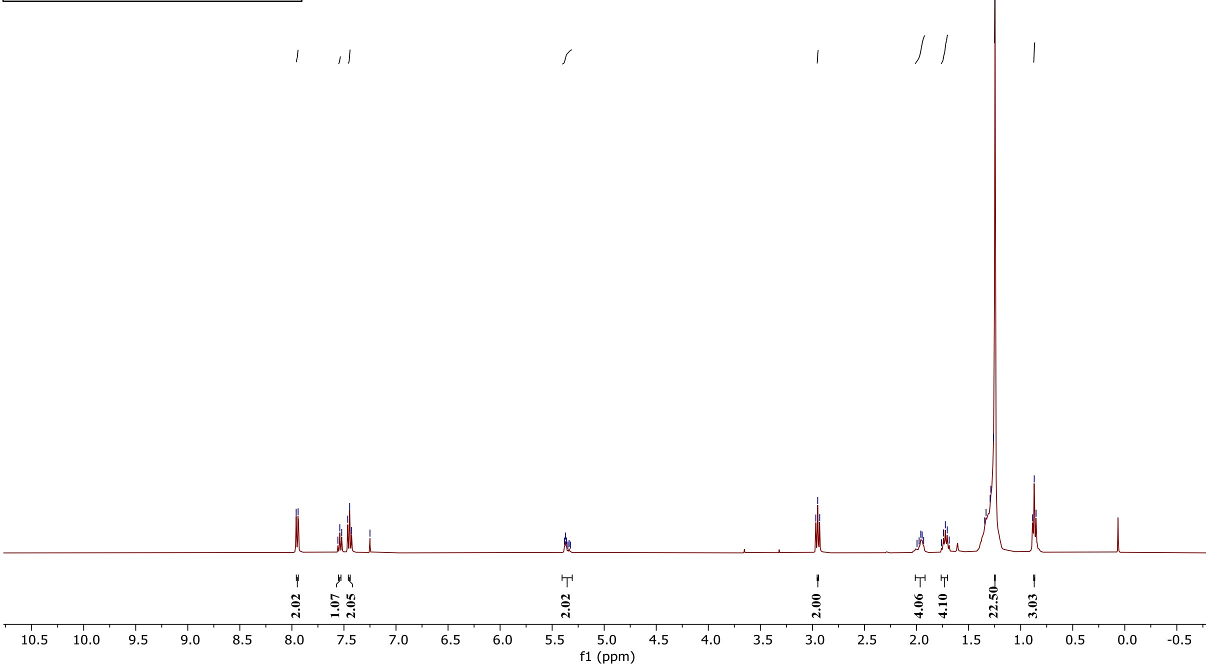


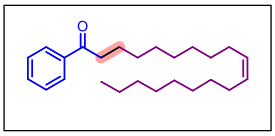
^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)



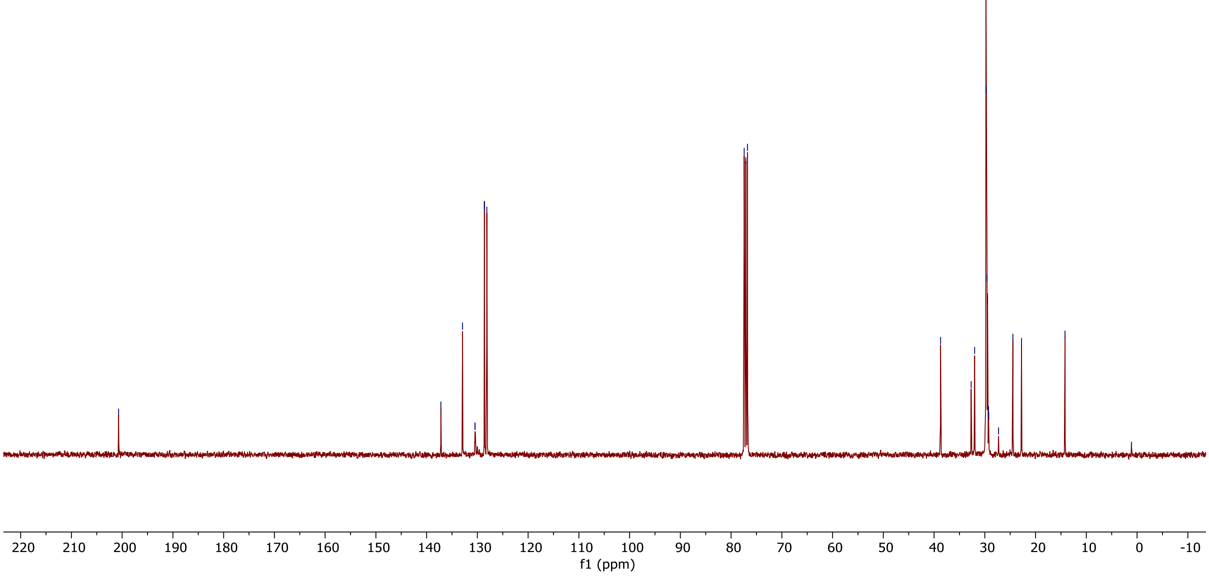


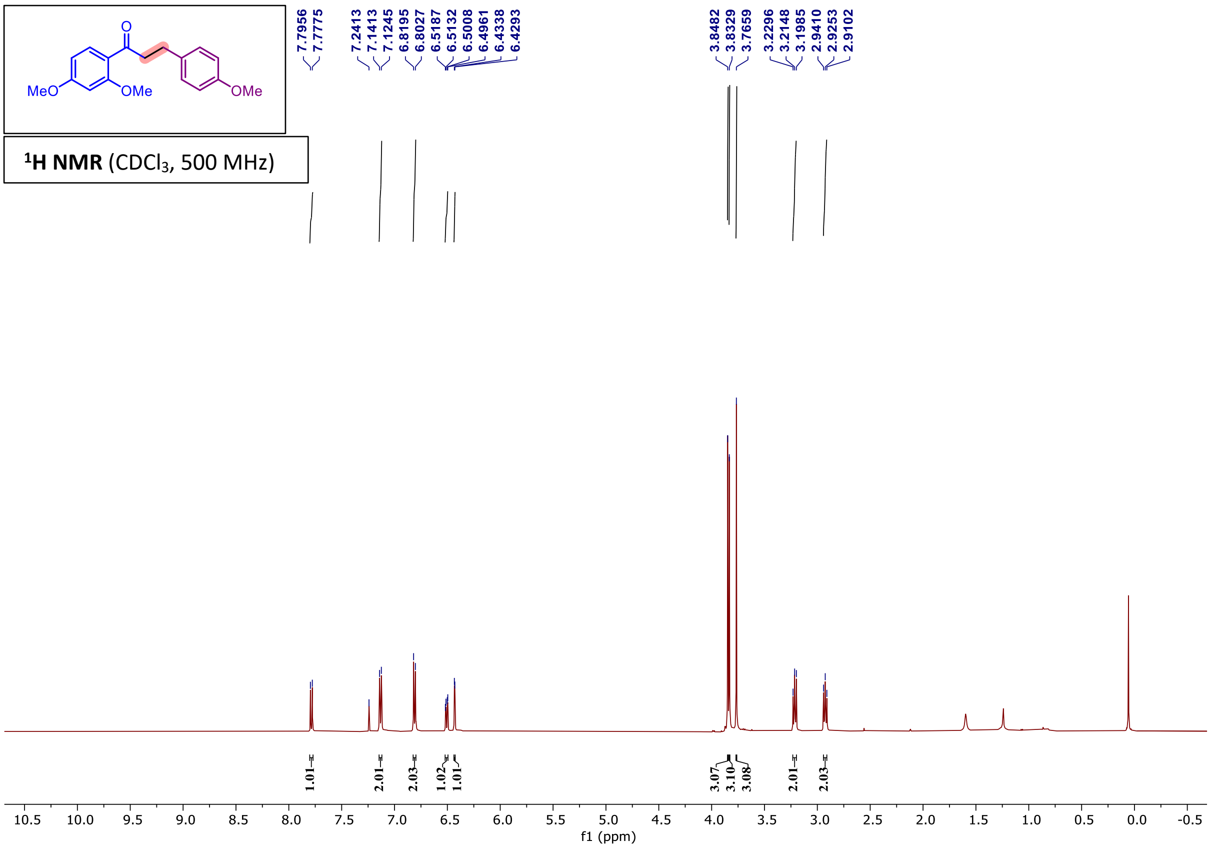
^{1}H NMR ($CDCl_3$, 400 MHz)

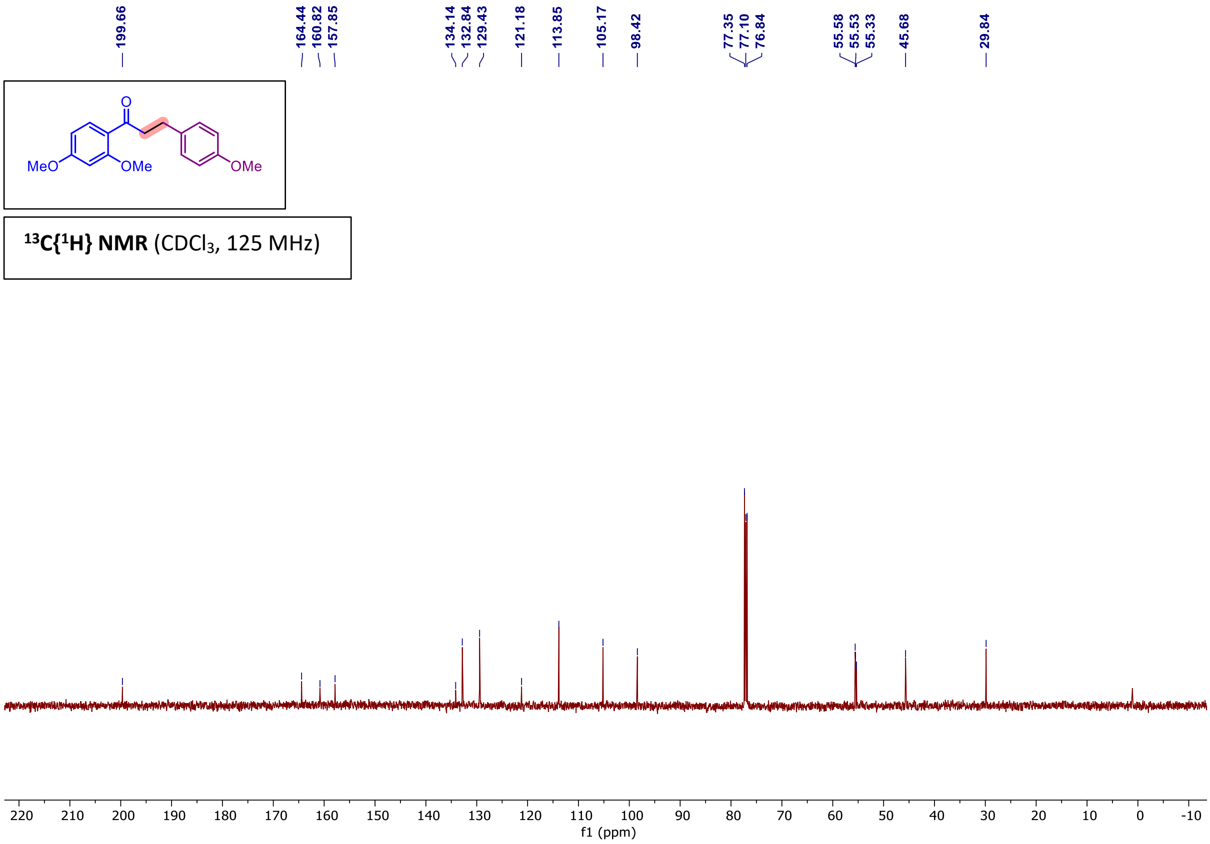


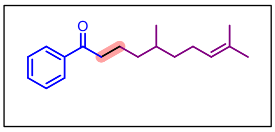


^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz)

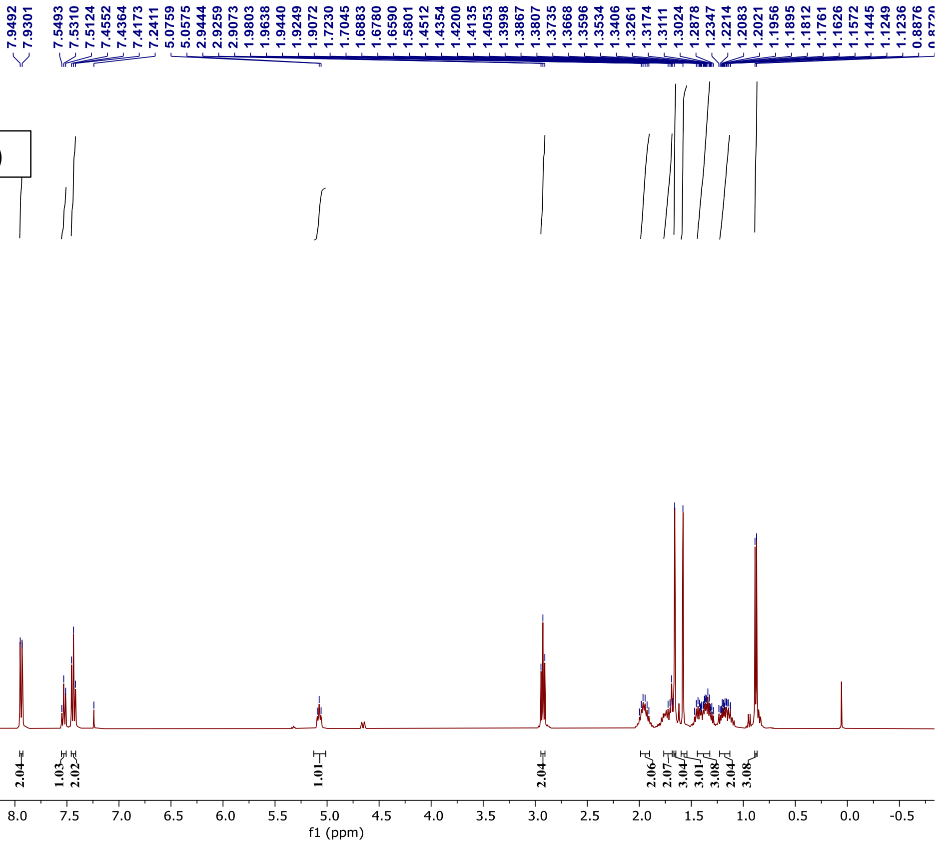


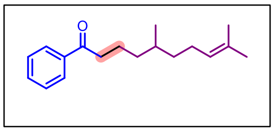

O
MeO
OMe
OMe
1H NMR (CDCl3, 500 MHz)
7.7956 7.7775 7.2413 7.1413 7.1245 6.8195 6.8027 6.5187 6.5132 6.5008 6.4961 6.4338 6.4293
3.8482 3.8329 3.7659 3.2296 3.2148 3.1985 2.9410 2.9253 2.9102
1.01 2.01 2.03 1.02 1.01 3.07 3.10 3.08 2.01 2.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


O
MeO
OMe
OMe
13C{1H} NMR (CDCl3, 125 MHz)
199.66 164.44 160.82 157.85 134.14 132.84 129.43 121.18 113.85 105.17 98.42 77.35 77.10 76.84 55.58 55.53 55.33 45.68 29.84
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

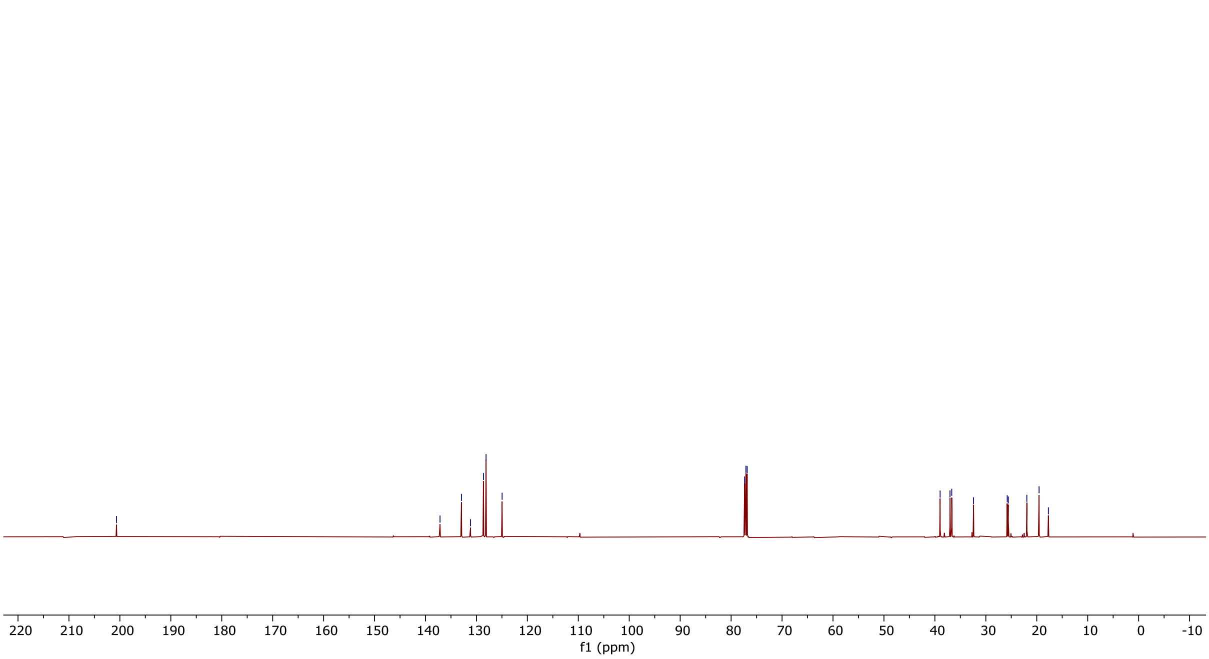


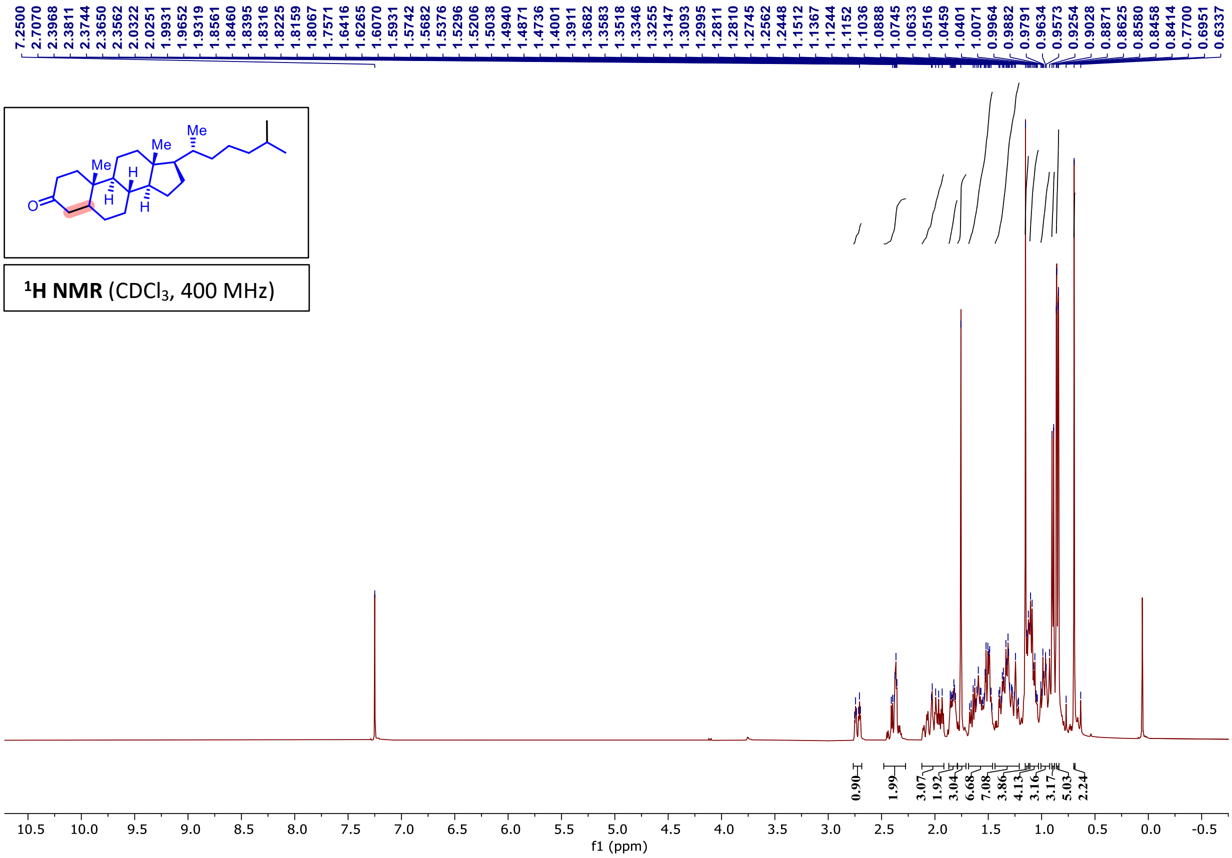
^{1}H NMR ($CDCl_3$, 400 MHz)

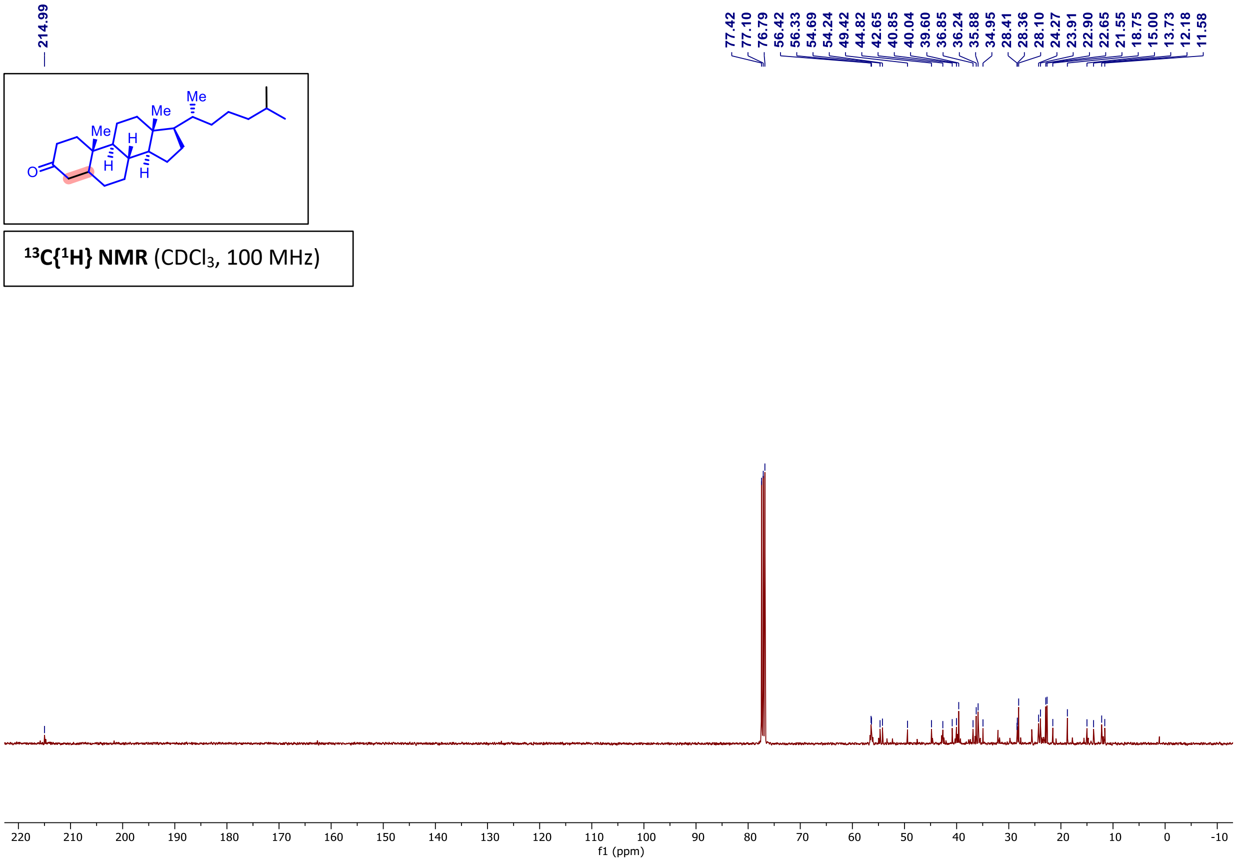


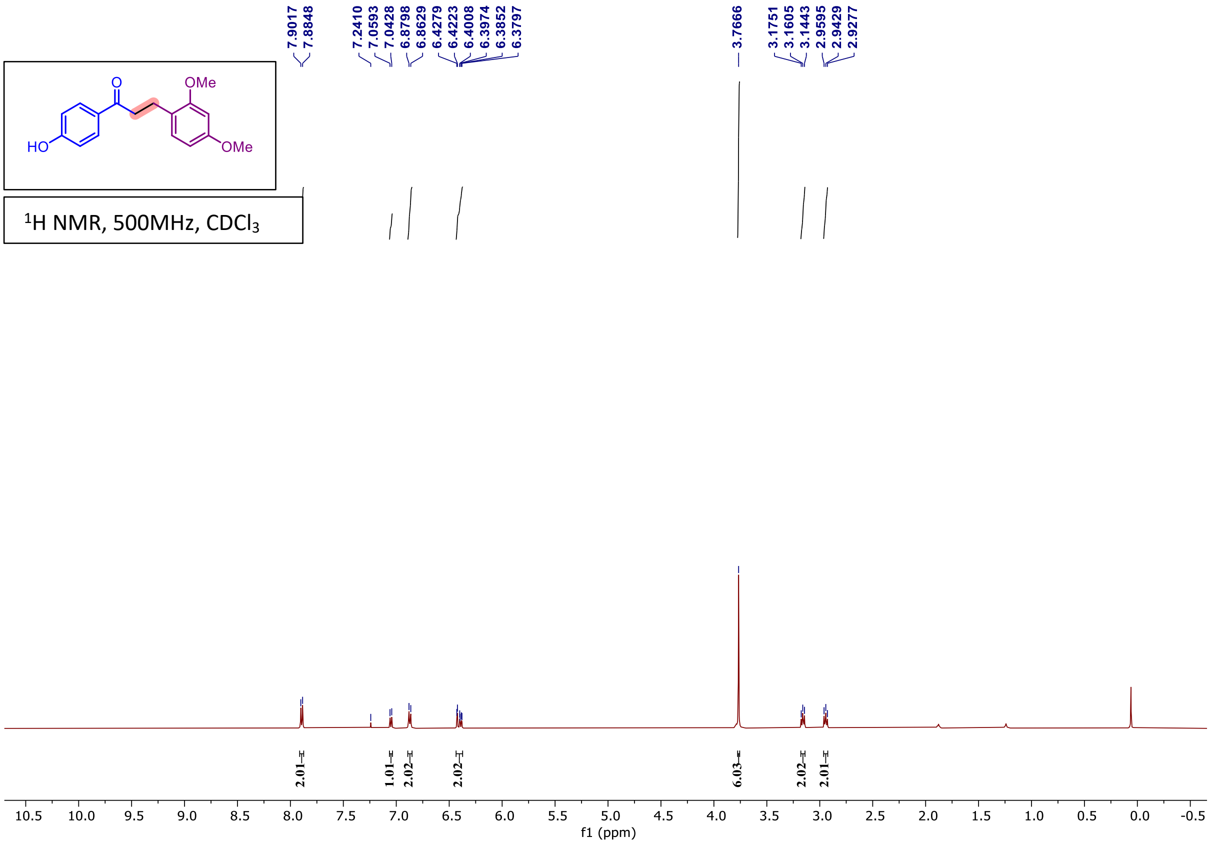


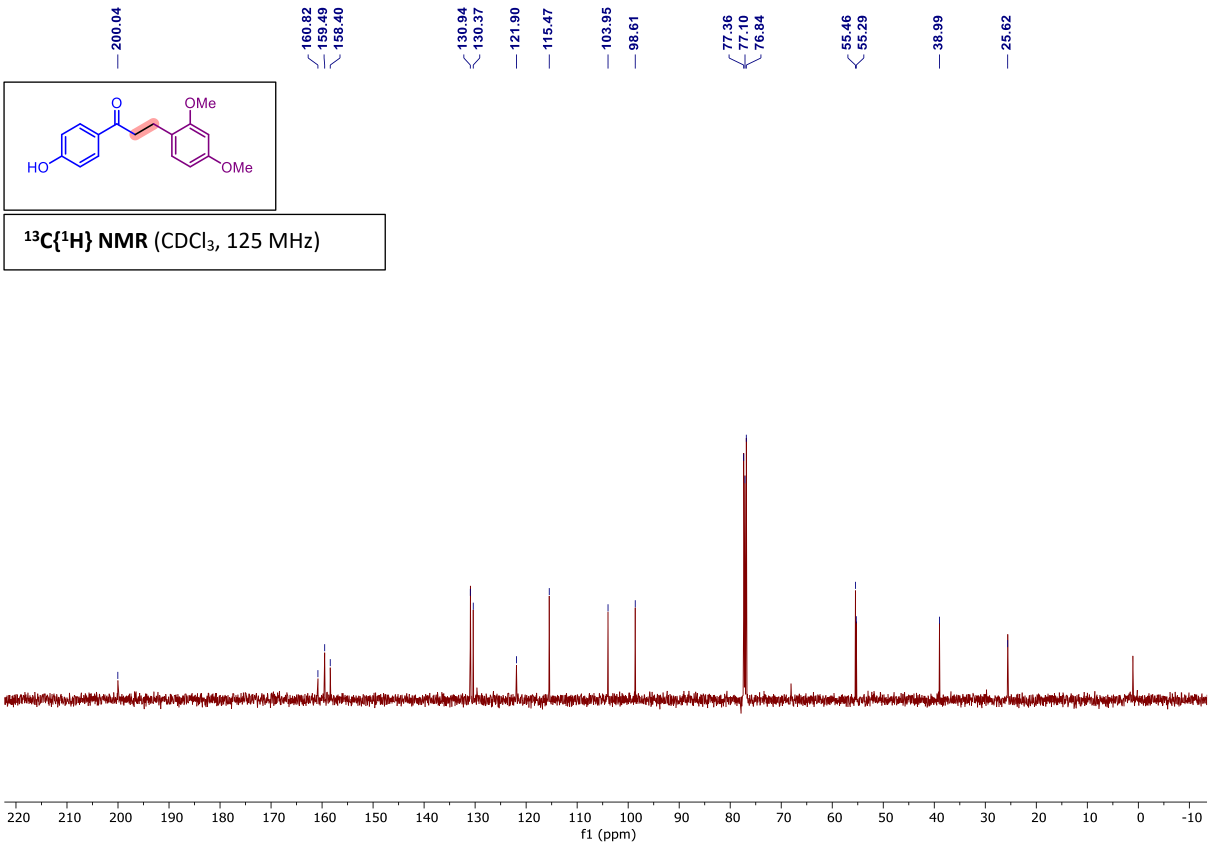
^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)

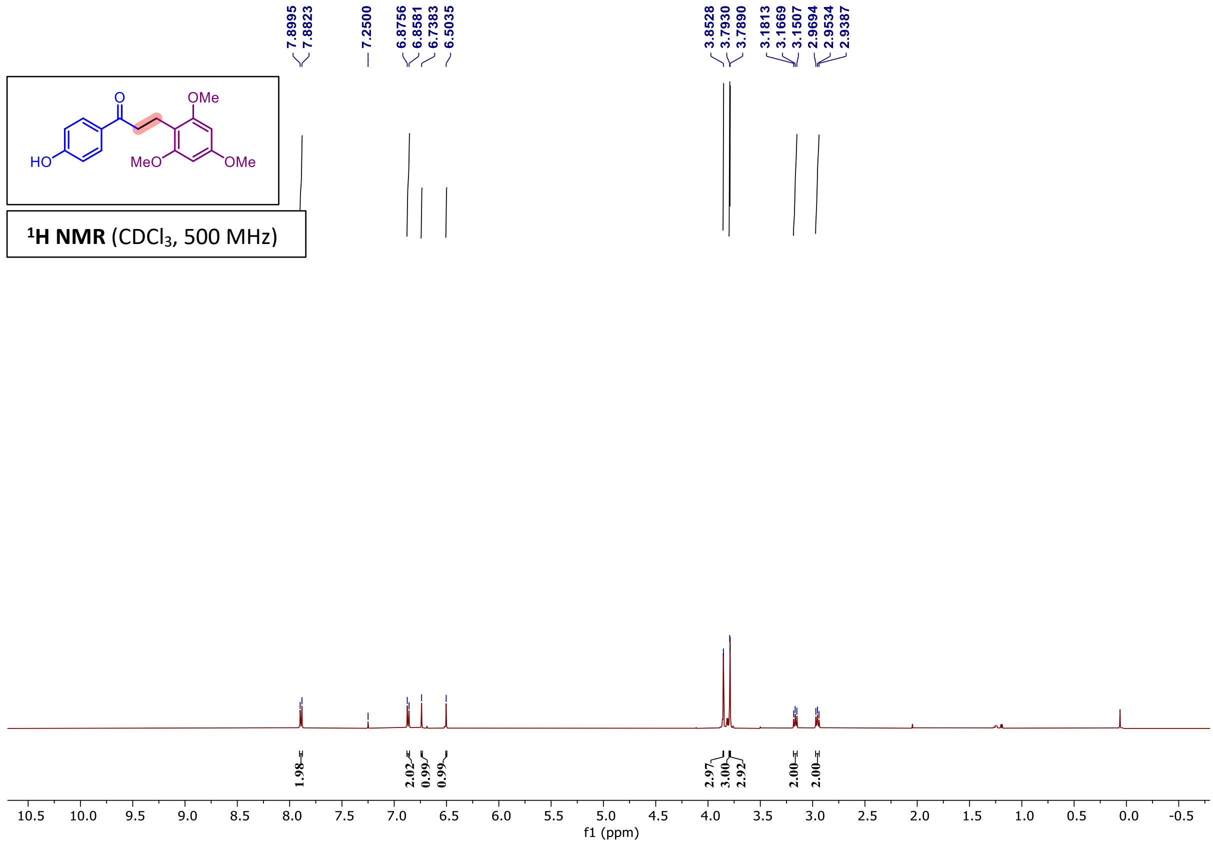



Me
Me
Me
H
H
H
O
¹H NMR (CDCl₃, 400 MHz)
f1 (ppm)

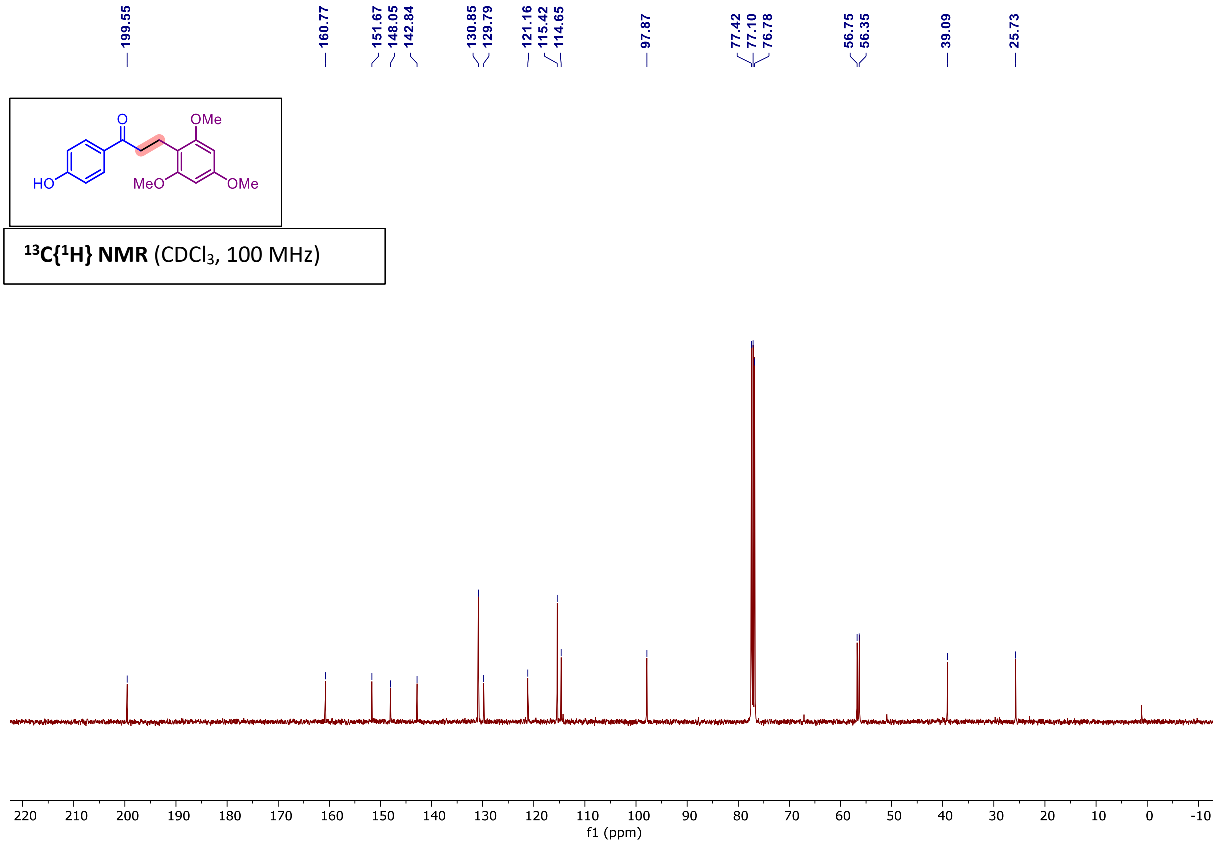

214.99
Me
Me
Me
H
H
H
O
¹³C{¹H} NMR (CDCl₃, 100 MHz)
f1 (ppm)


7.9017
7.8848
7.2410
7.0593
7.0428
6.8798
6.8629
6.4279
6.4223
6.4008
6.3974
6.3852
6.3797
3.7666
3.1751
3.1605
3.1443
2.9595
2.9429
2.9277
O
OMe
HO
OMe
¹H NMR, 500MHz, CDCl₃
2.01
1.01
2.02
2.02
6.03
2.02
2.01
f1 (ppm)

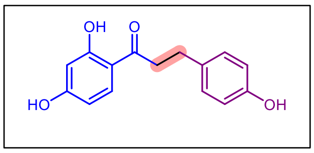

200.04
160.82
159.49
158.40
130.94
130.37
121.90
115.47
103.95
98.61
77.36
77.10
76.84
55.46
55.29
38.99
25.62
O
OMe
HO
OMe
¹³C{¹H} NMR (CDCl₃, 125 MHz)
f1 (ppm)



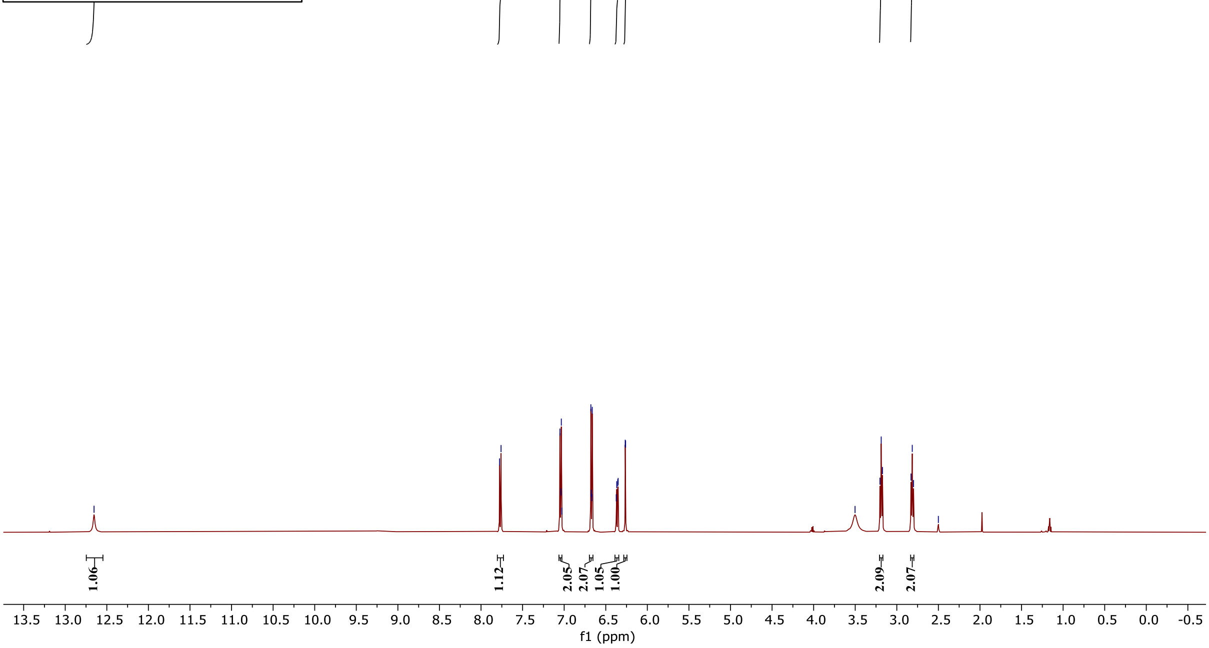
^{1}H NMR (CDCl$_3$, 500 MHz)

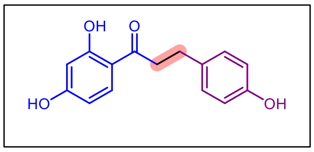


^{13}C{^{1}H} NMR (CDCl$_3$, 100 MHz)

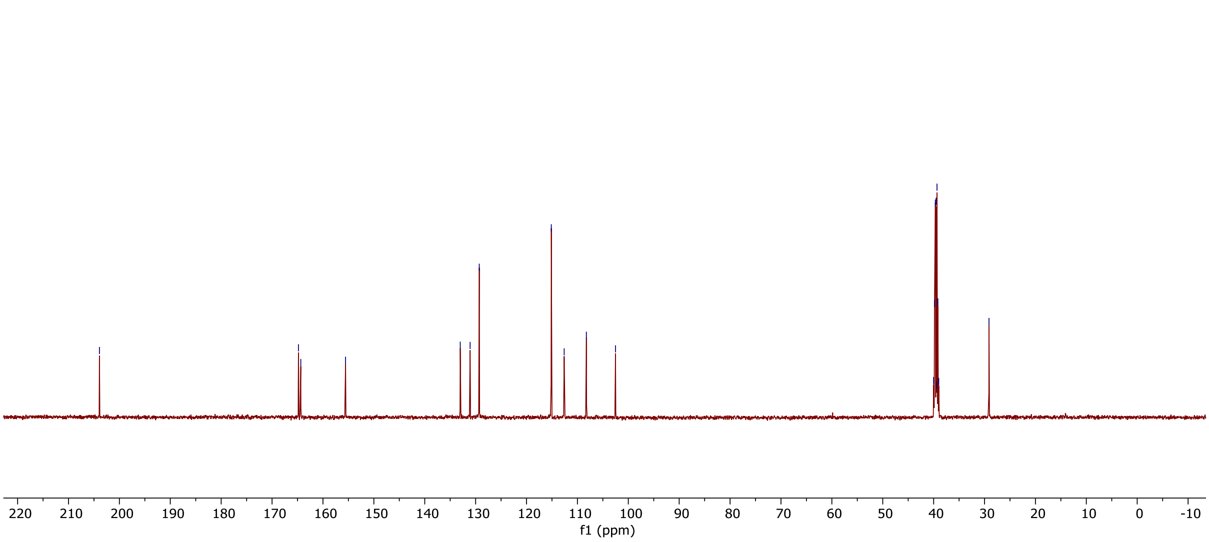


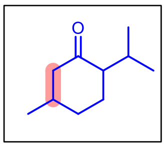
¹H NMR ($CDCl_3$, 500 MHz)



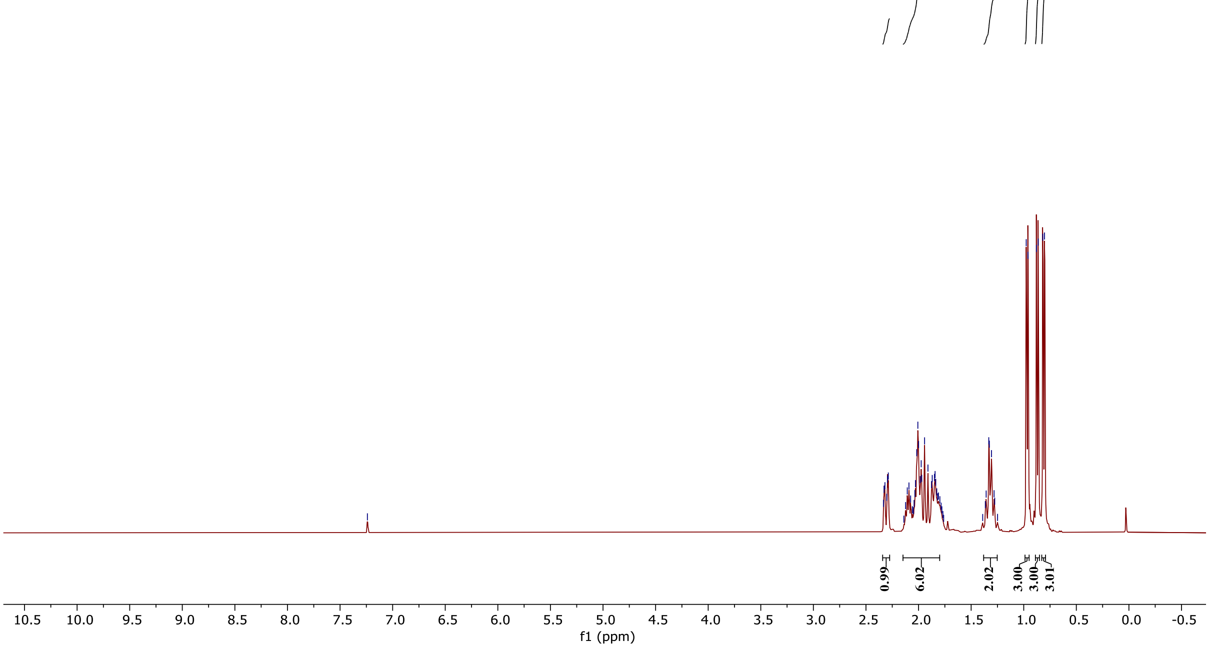


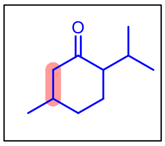
¹³C{¹H} NMR ($CDCl_3$, 125 MHz)



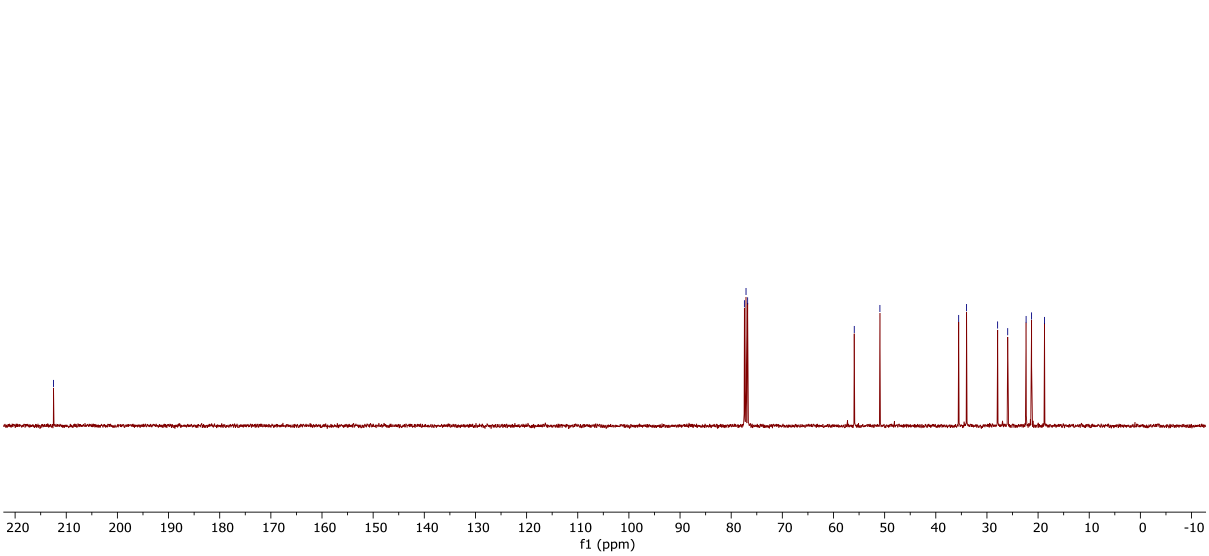


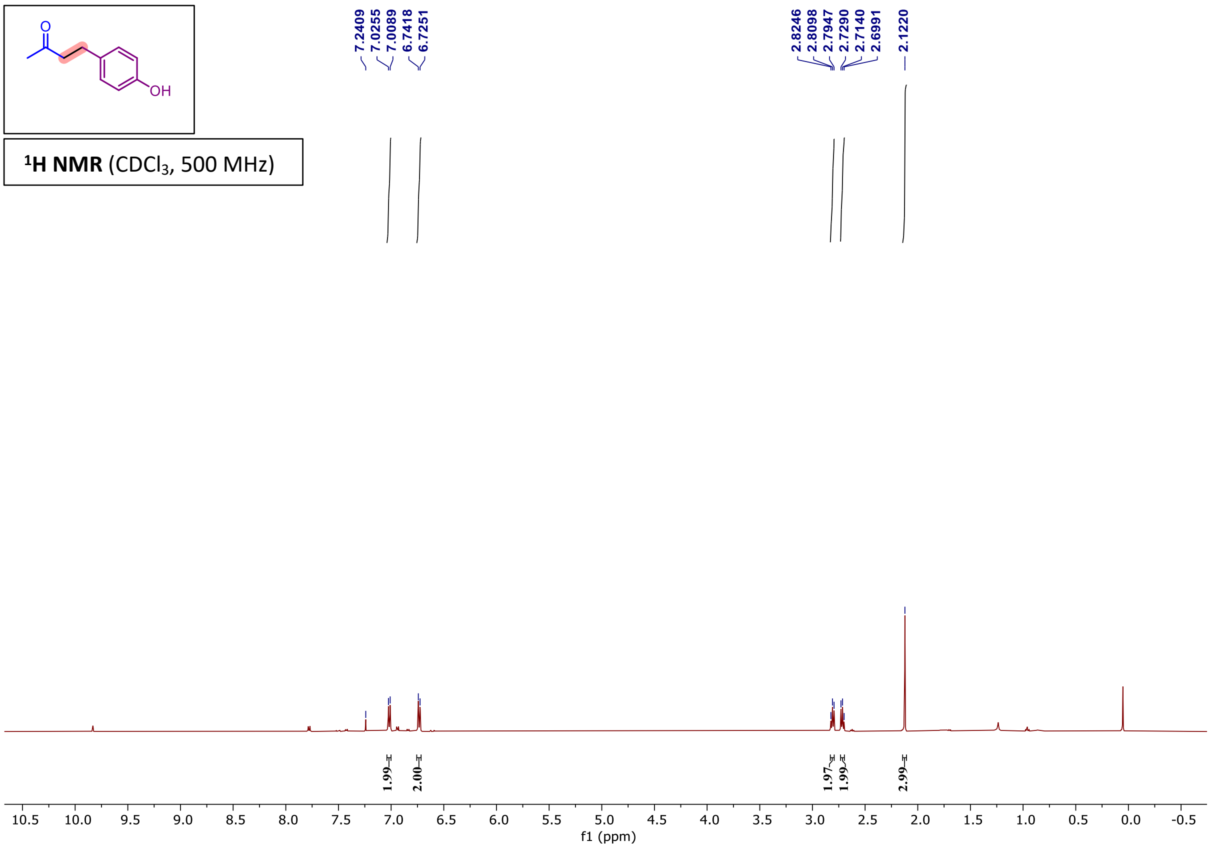
^{1}H NMR ($CDCl_3$, 400 MHz)



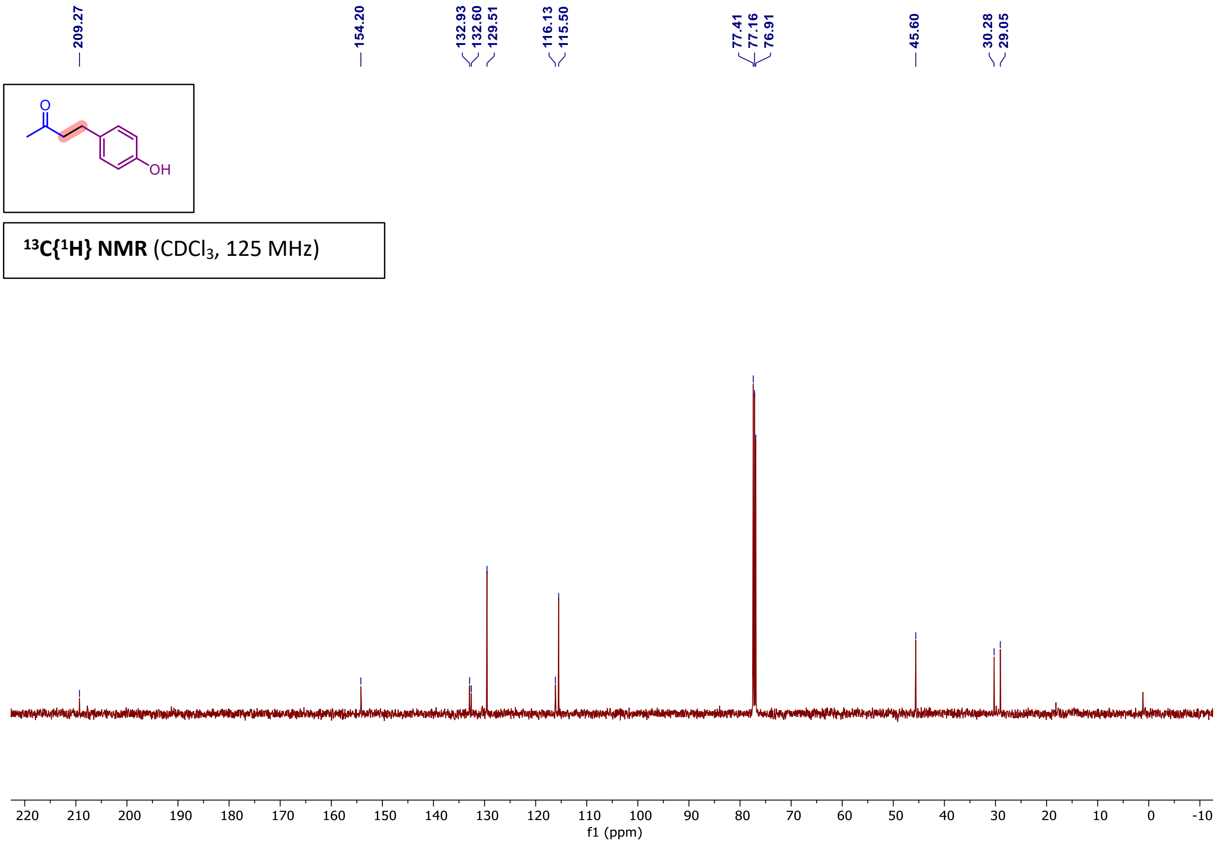


$^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz)

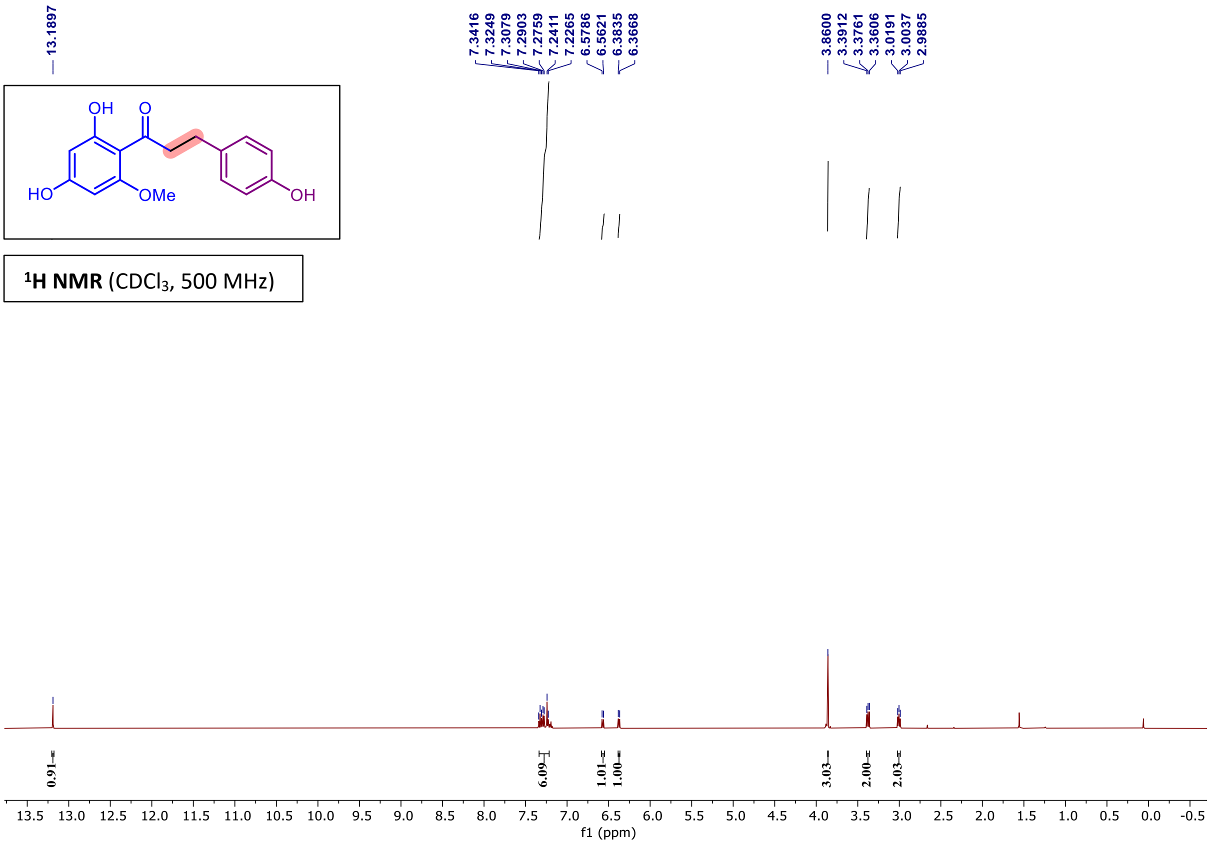


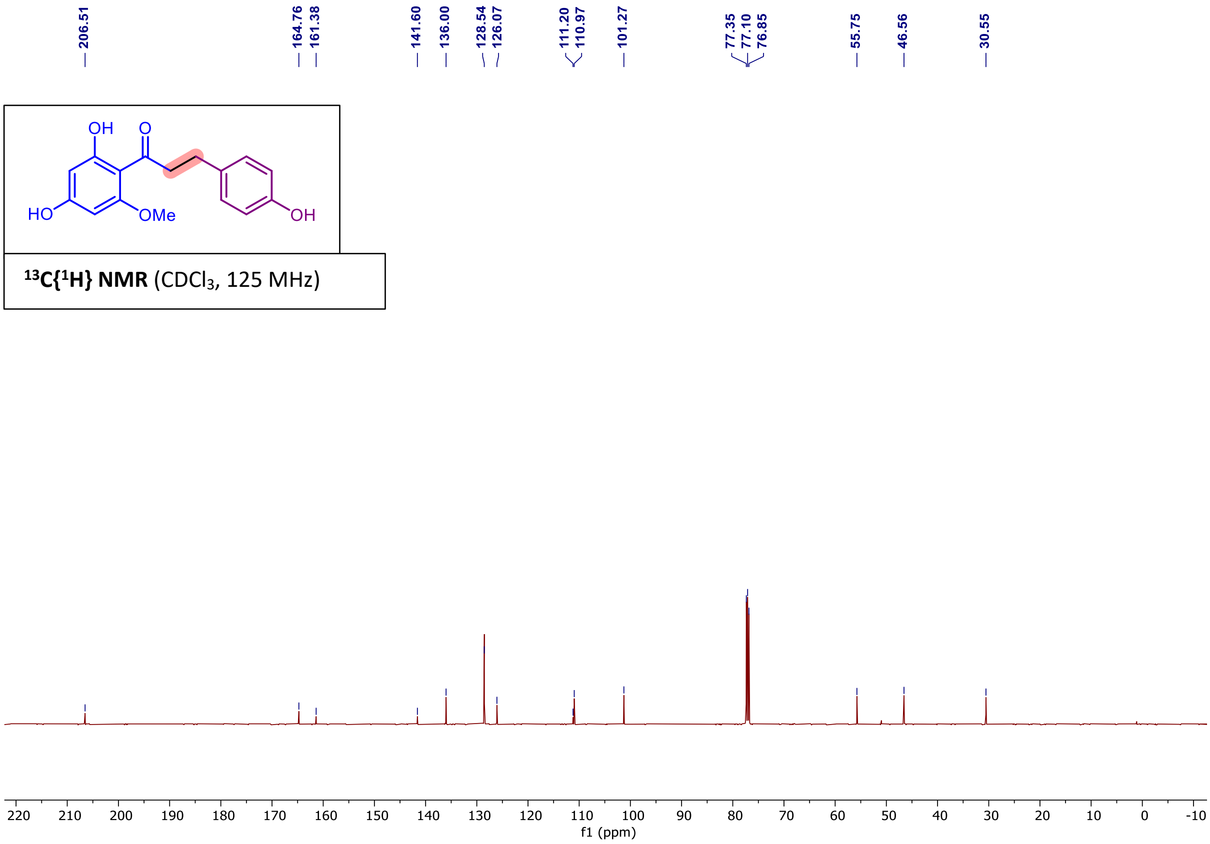


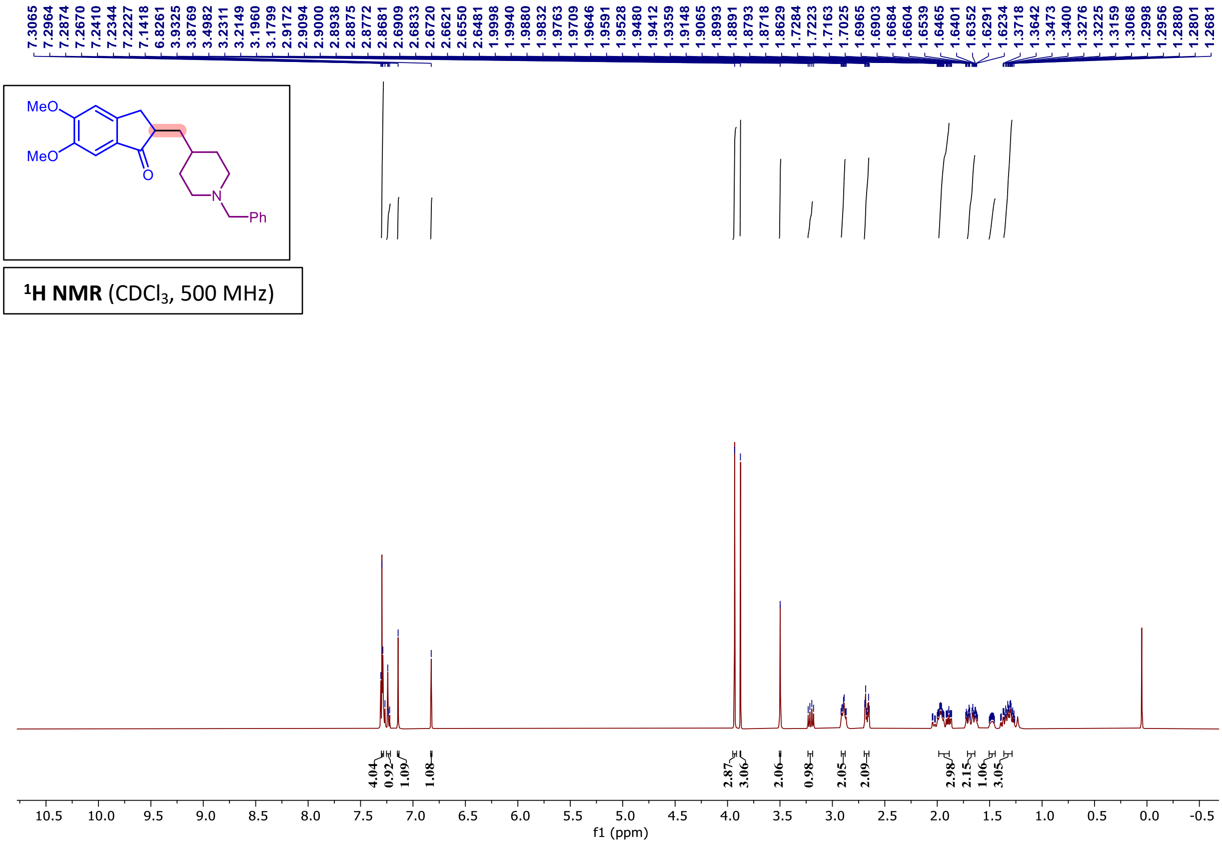
OH
O
1H NMR (CDCl3, 500 MHz)
7.2409
7.0255
7.0089
6.7418
6.7251
2.8246
2.8098
2.7947
2.7290
2.7140
2.6991
2.1220
1.99
2.00
1.97
1.99
2.99
f1 (ppm)



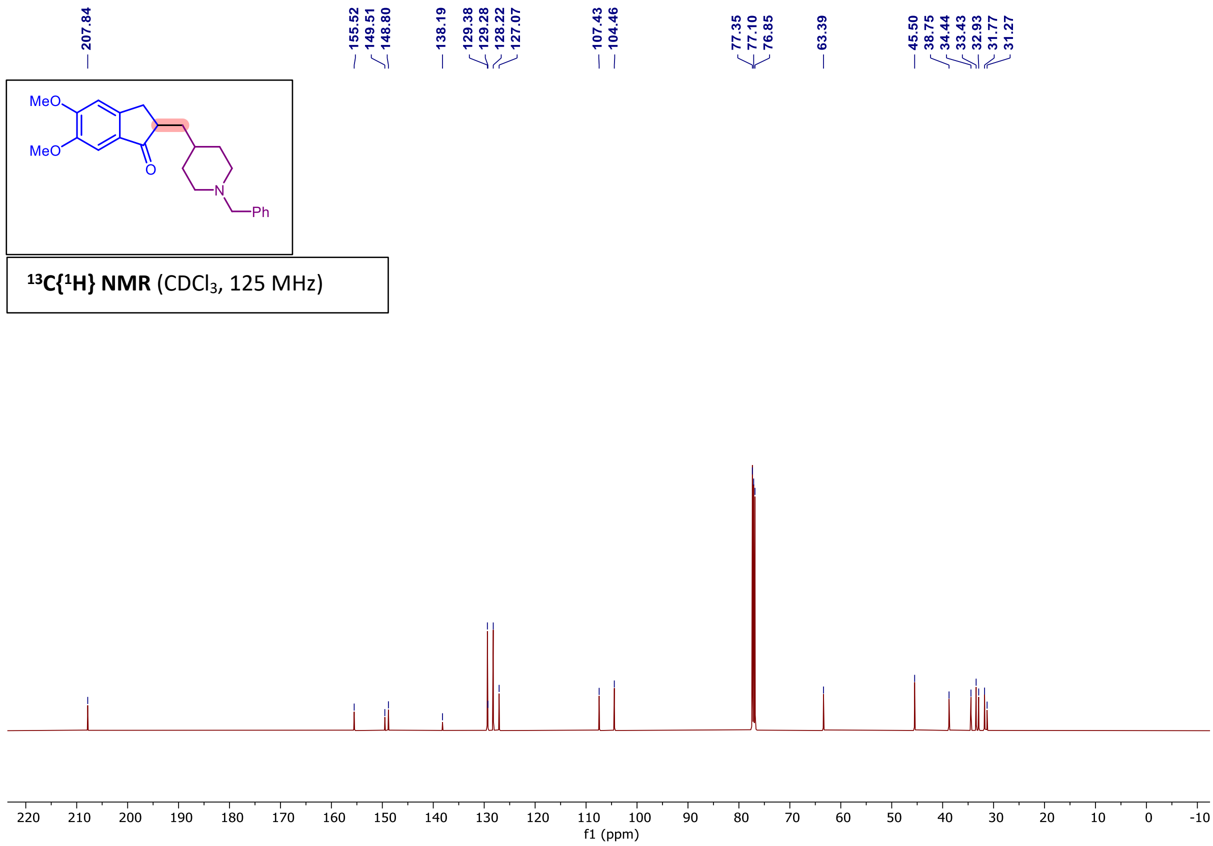
OH
O
13C{1H} NMR (CDCl3, 125 MHz)
209.27
154.20
132.93
132.60
129.51
116.13
115.50
77.41
77.16
76.91
45.60
30.28
29.05
f1 (ppm)


13.1897
7.3416 7.3249 7.3079 7.2903 7.2759 7.2411 7.2265 6.5786 6.5621 6.3835 6.3668
3.8600 3.3912 3.3761 3.3606 3.0191 3.0037 2.9885
OH O
HO OMe OH
¹H NMR (CDCl₃, 500 MHz)
0.91 6.09 1.01 1.00 3.03 2.00 2.03
f1 (ppm)

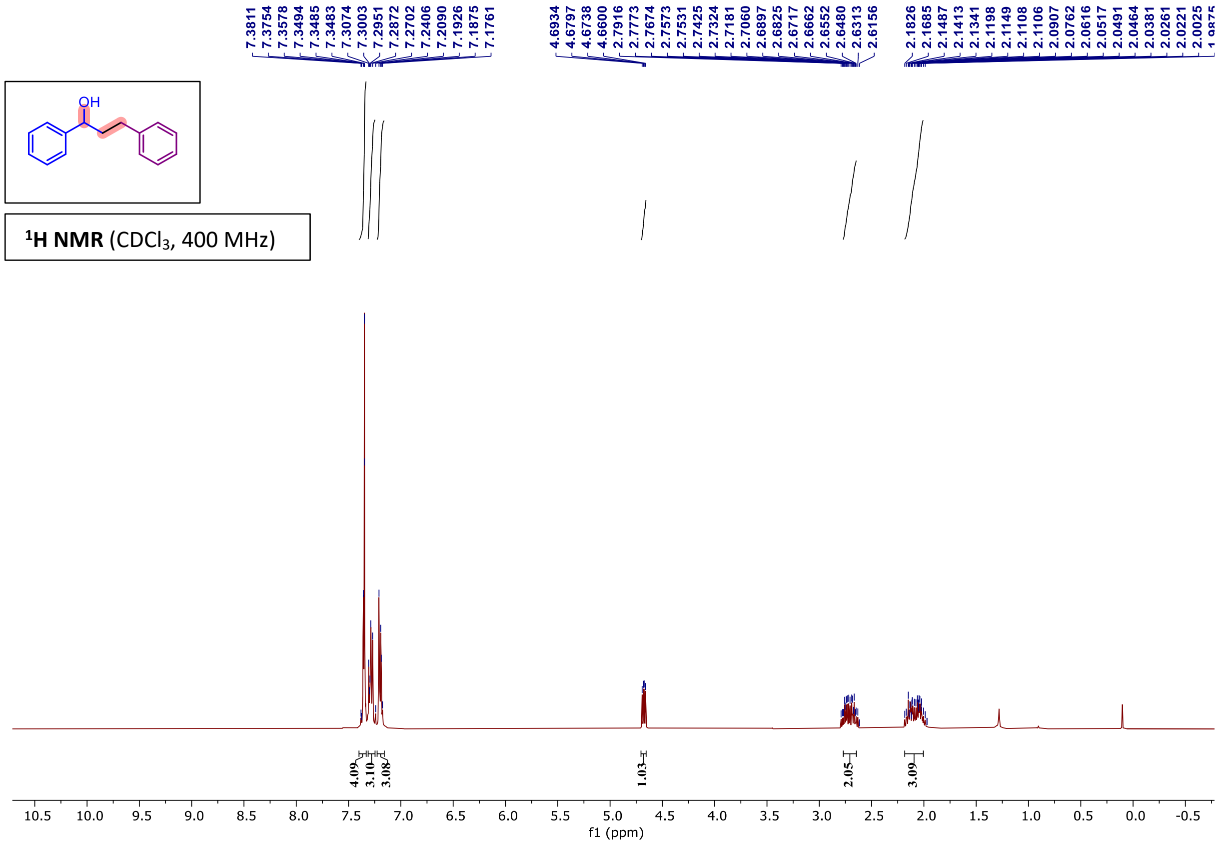

206.51
164.76 161.38
141.60 136.00 128.54 126.07
111.20 110.97 101.27
77.35 77.10 76.85
55.75 46.56 30.55
OH O
HO OMe OH
¹³C{¹H} NMR (CDCl₃, 125 MHz)
f1 (ppm)

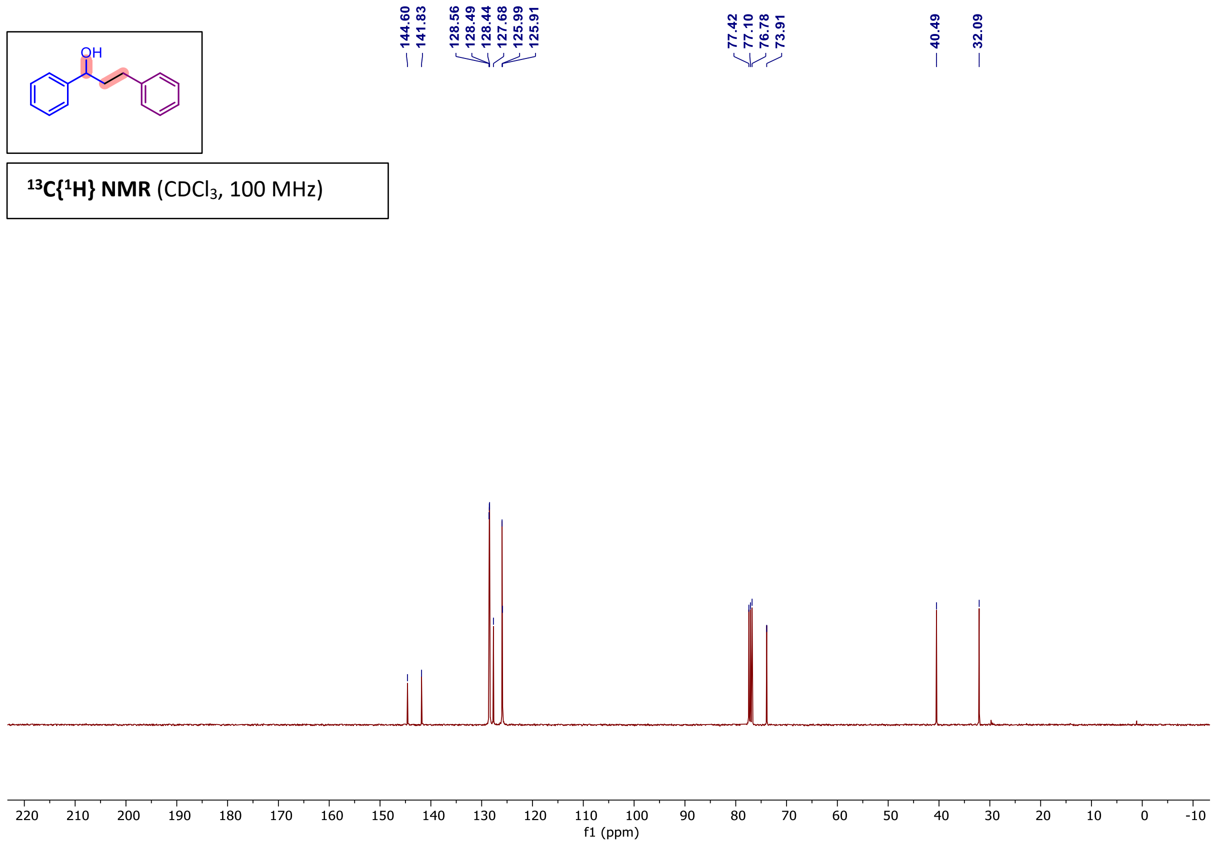


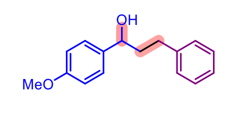
^{1}H NMR ($CDCl_3$, 500 MHz)



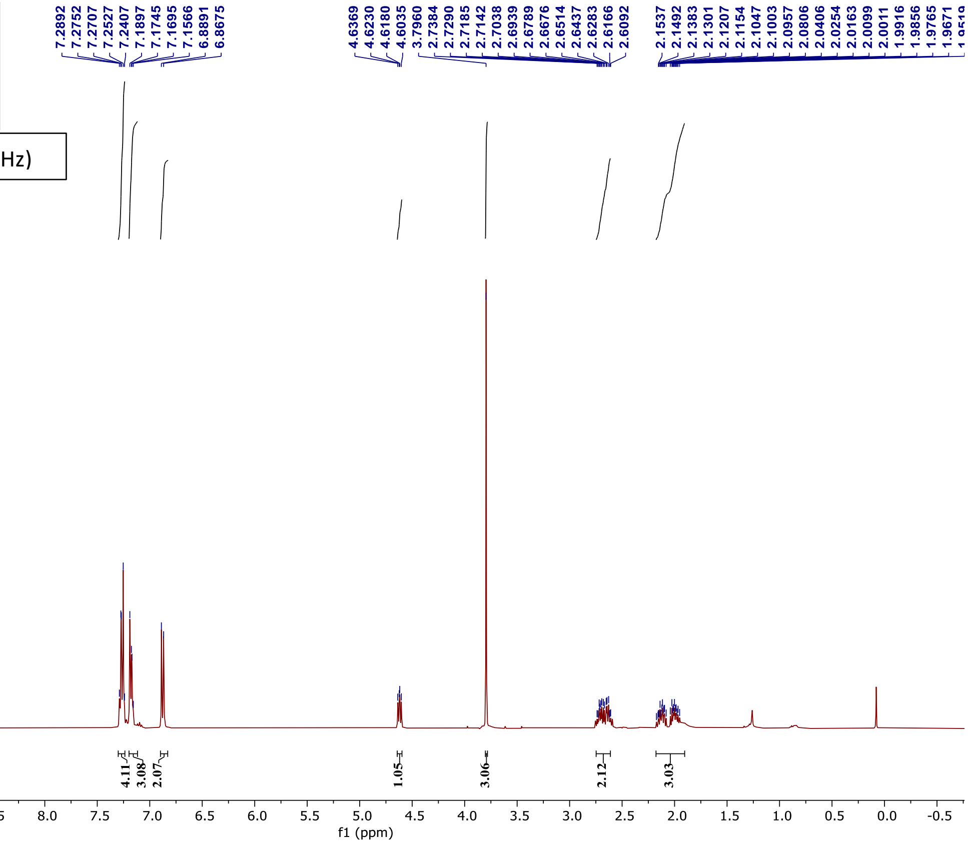
$^{13}C\{^1H\}$ NMR ($CDCl_3$, 125 MHz)

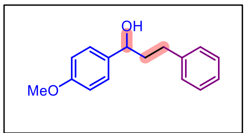

OH
¹H NMR (CDCl₃, 400 MHz)
f1 (ppm)


OH
¹³C{¹H} NMR (CDCl₃, 100 MHz)
144.60
141.83
128.56
128.49
128.44
127.68
125.99
125.91
77.42
77.10
76.78
73.91
40.49
32.09
f1 (ppm)

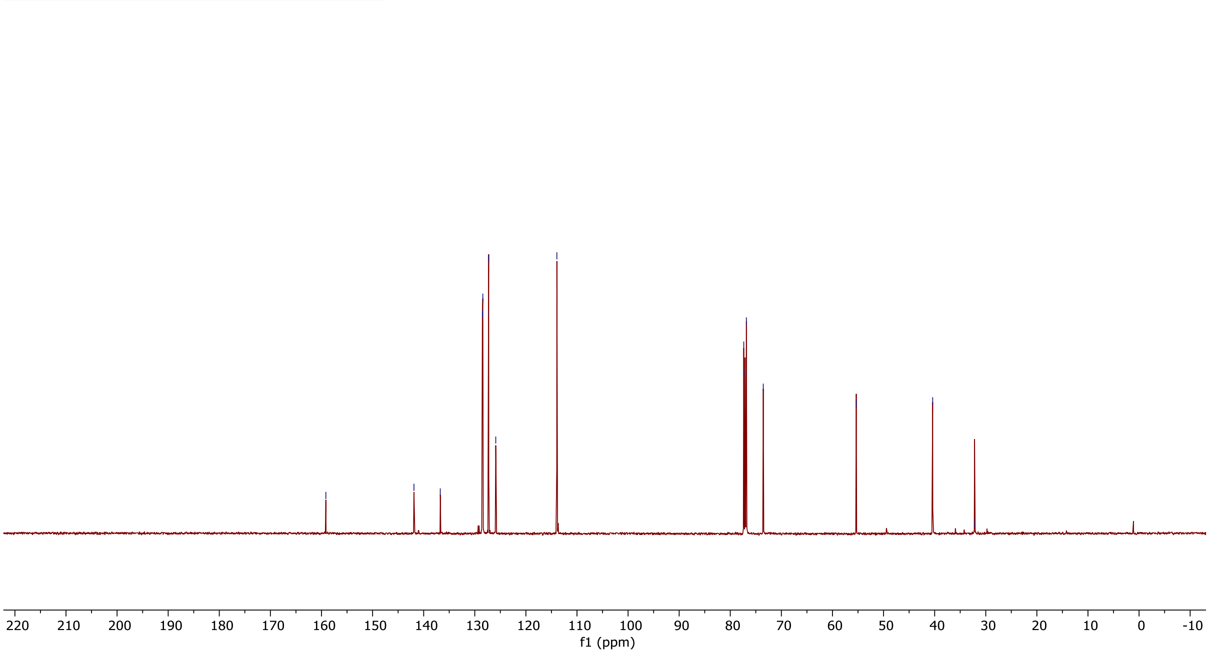


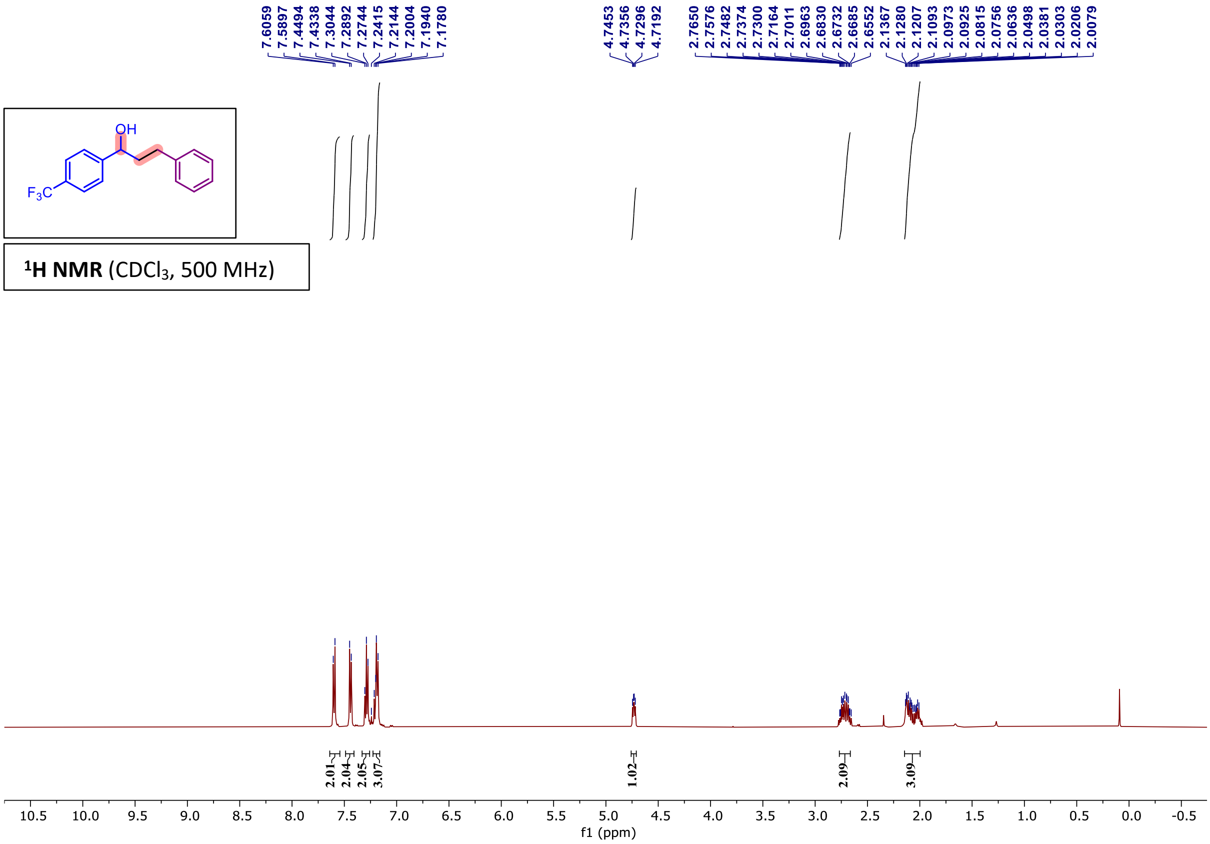
^{1}H NMR ($CDCl_3$, 400 MHz)



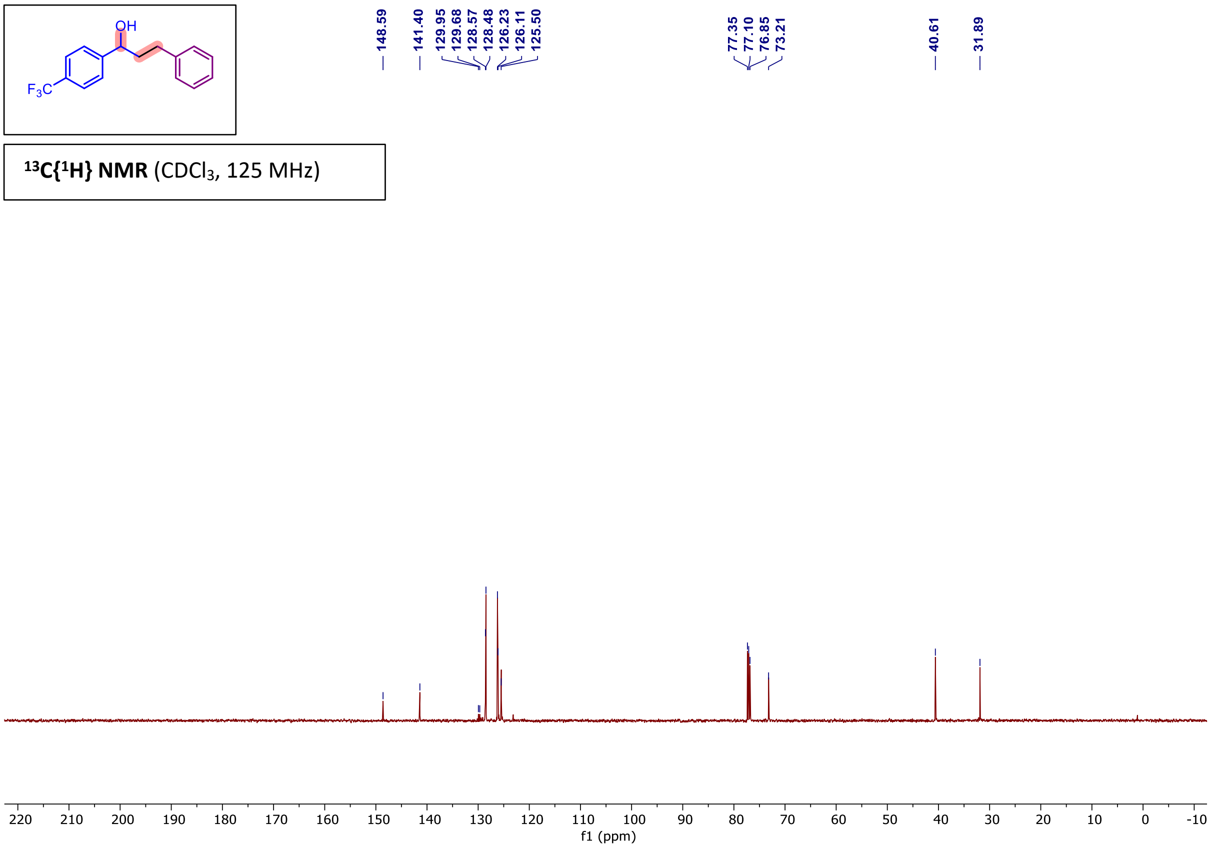


^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)

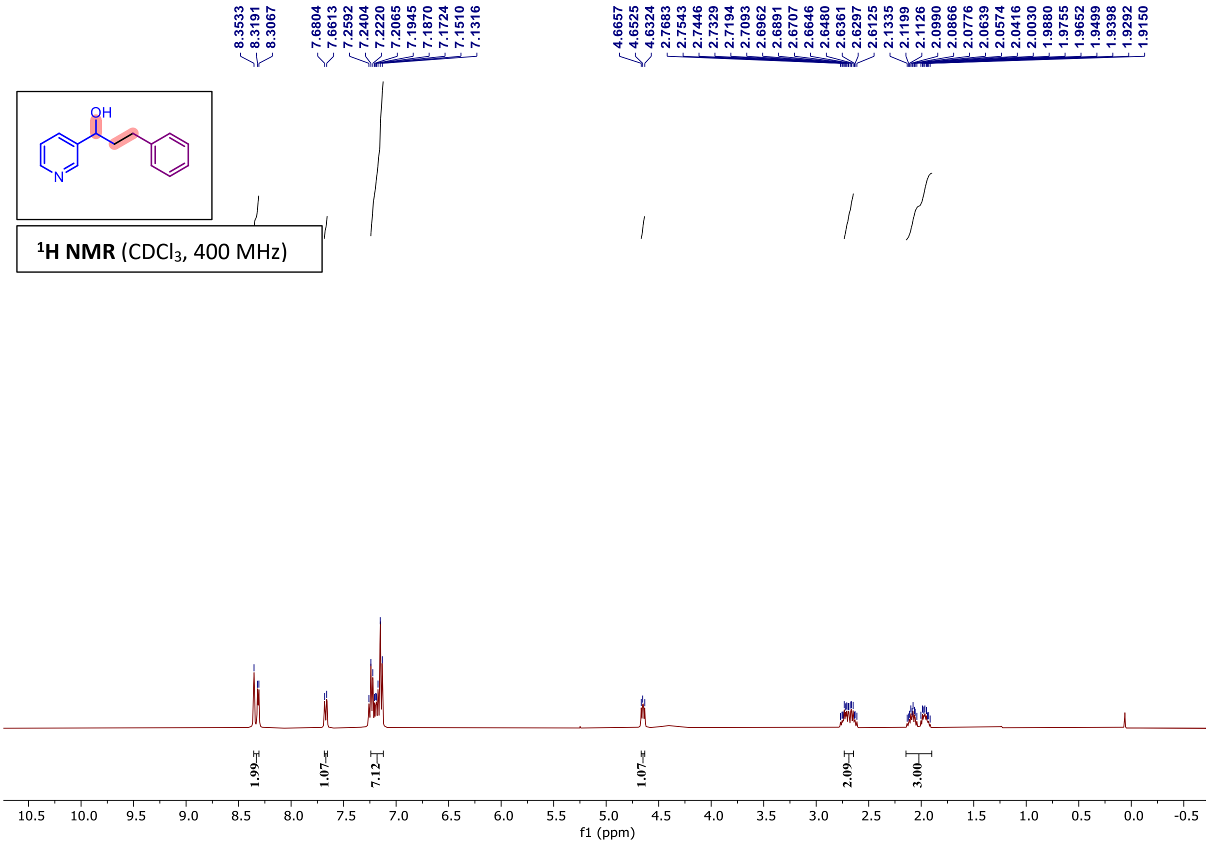


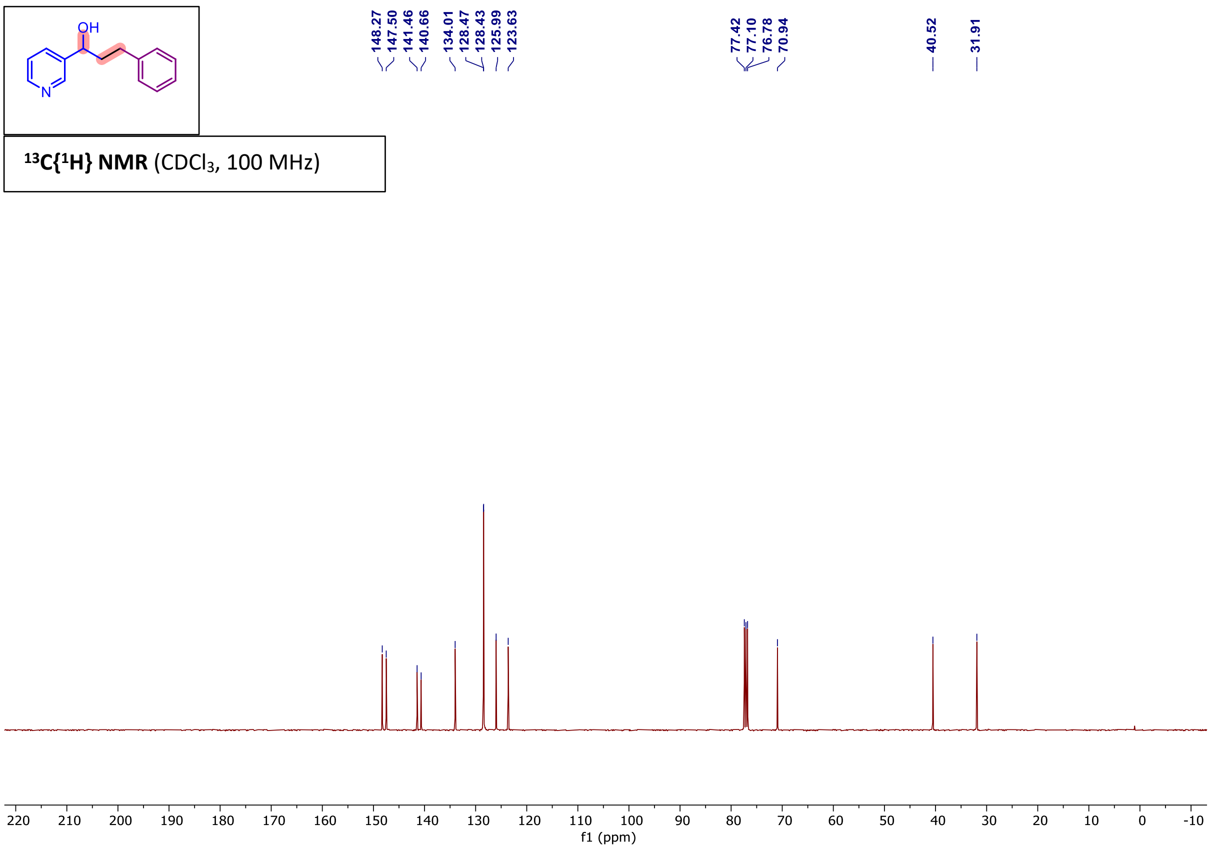


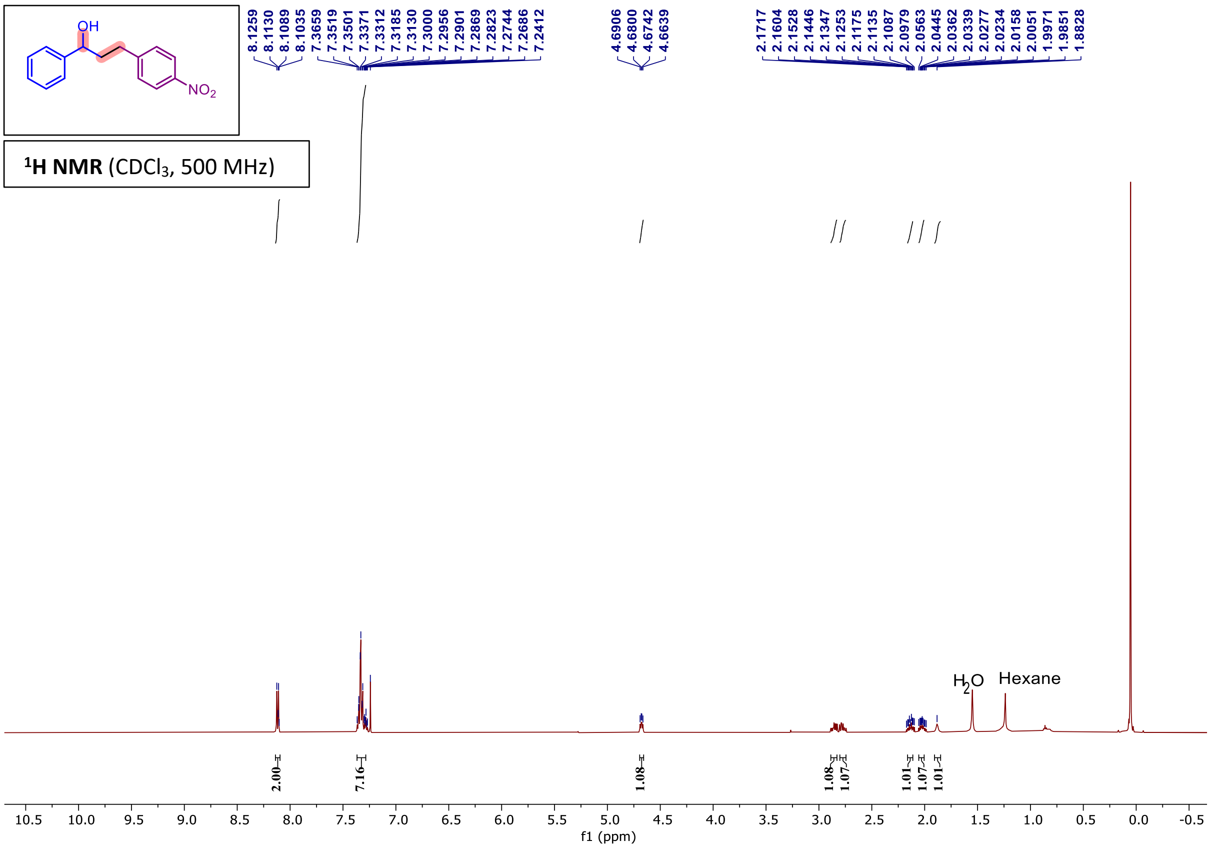
^{1}H NMR ($CDCl_3$, 500 MHz)

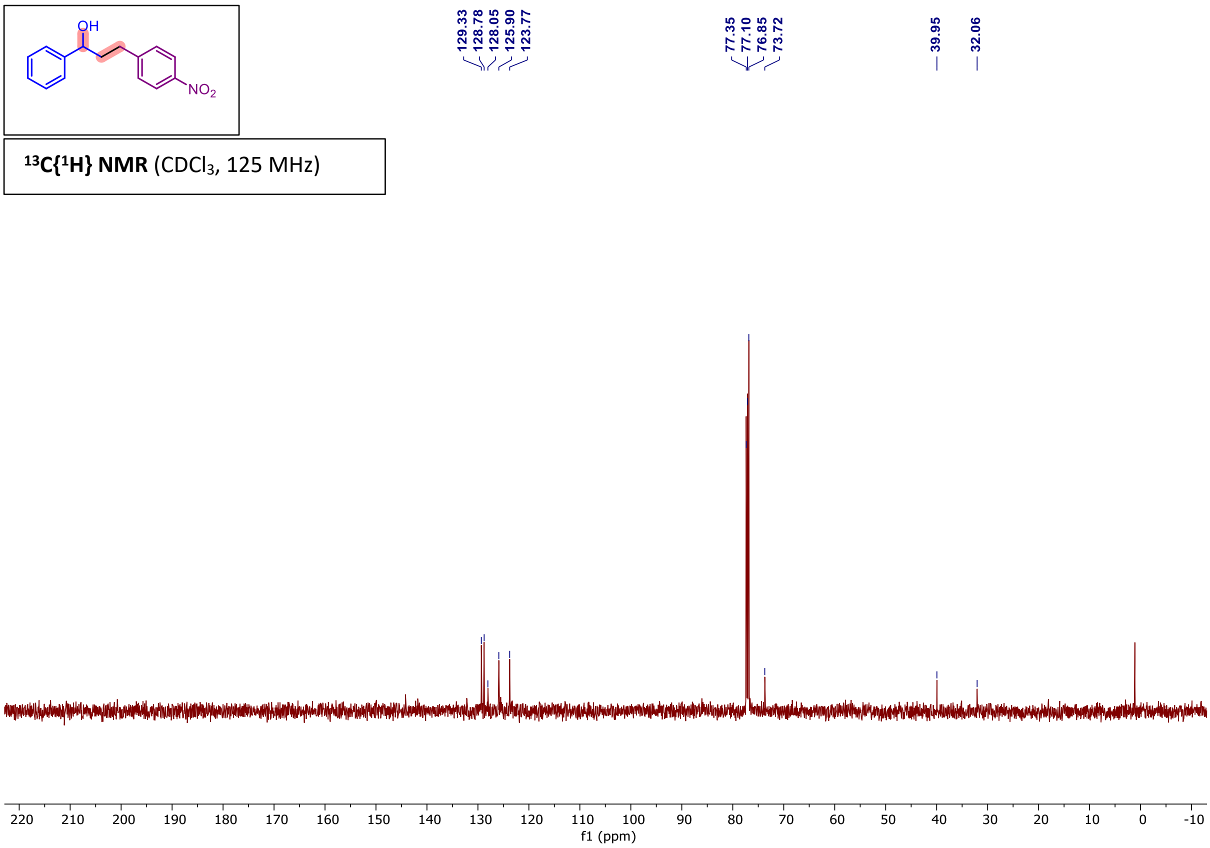


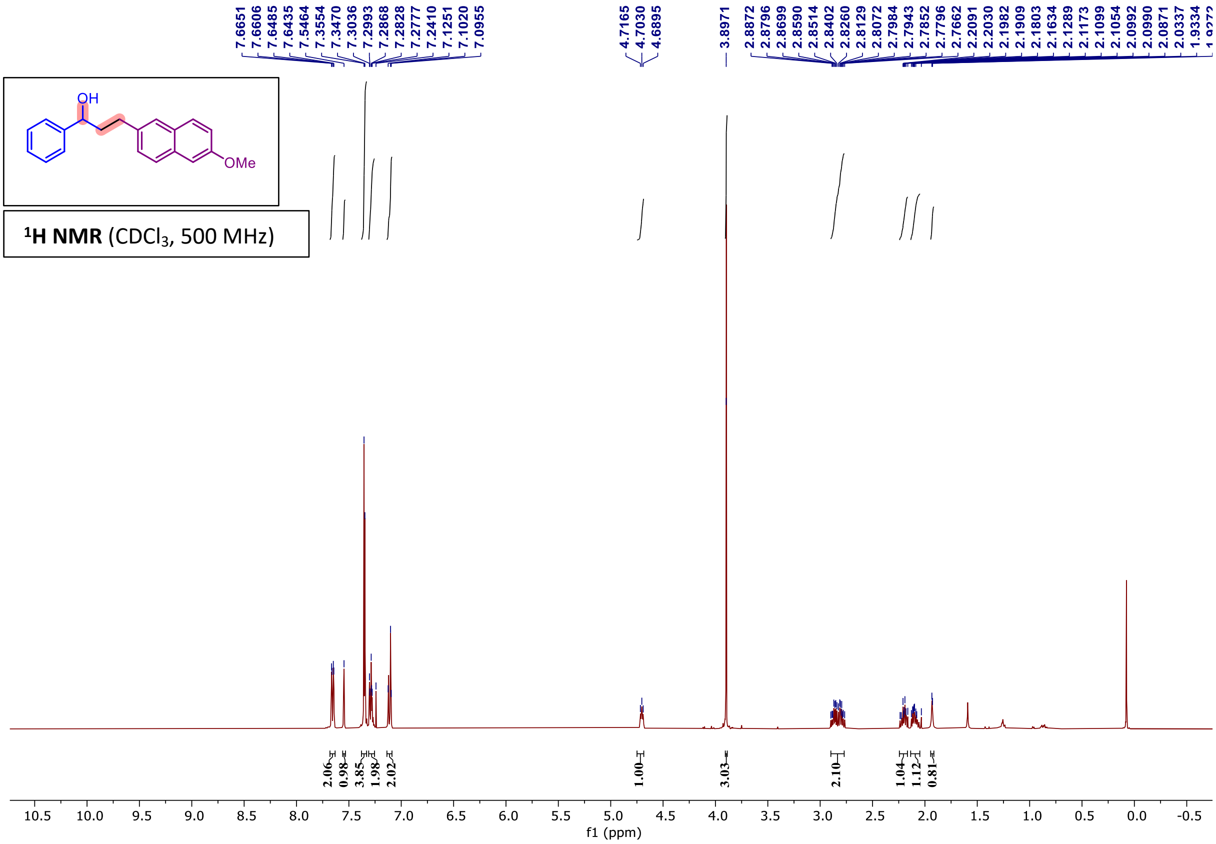
^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)

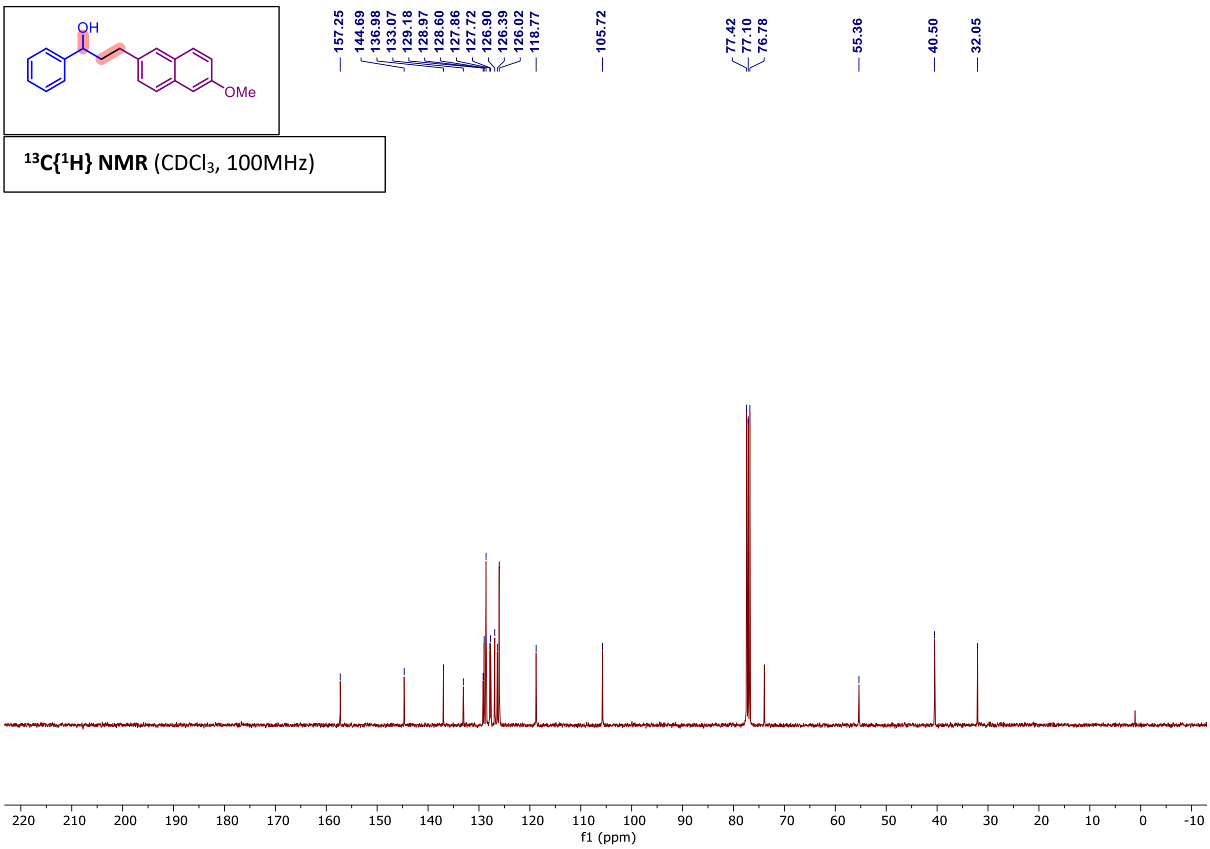

OH
N
¹H NMR (CDCl₃, 400 MHz)
8.3533
8.3191
8.3067
7.6804
7.6613
7.2592
7.2404
7.2220
7.2065
7.1945
7.1870
7.1724
7.1510
7.1316
4.6657
4.6525
4.6324
2.7683
2.7543
2.7446
2.7329
2.7194
2.7093
2.6962
2.6891
2.6707
2.6646
2.6480
2.6361
2.6297
2.6125
2.1335
2.1199
2.1126
2.0990
2.0866
2.0776
2.0639
2.0574
2.0416
2.0030
1.9880
1.9755
1.9652
1.9499
1.9398
1.9292
1.9150
1.99
1.07
7.12
1.07
2.09
3.00
f1 (ppm)

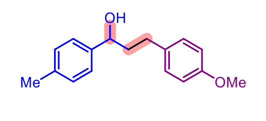

OH
N
¹³C{¹H} NMR (CDCl₃, 100 MHz)
148.27
147.50
141.46
140.66
134.01
128.47
128.43
125.99
123.63
77.42
77.10
76.78
70.94
40.52
31.91
f1 (ppm)


OH
NO2
¹H NMR (CDCl3, 500 MHz)
8.1259 8.1130 8.1089 8.1035 7.3659 7.3519 7.3501 7.3371 7.3312 7.3185 7.3130 7.3000 7.2956 7.2901 7.2869 7.2823 7.2744 7.2686 7.2412
4.6906 4.6800 4.6742 4.6639
2.1717 2.1604 2.1528 2.1446 2.1347 2.1253 2.1175 2.1135 2.1087 2.0979 2.0563 2.0445 2.0362 2.0339 2.0277 2.0234 2.0158 2.0051 1.9971 1.9851 1.8828
H2O
Hexane
2.00
7.16
1.08
1.08
1.07
1.01
1.07
1.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

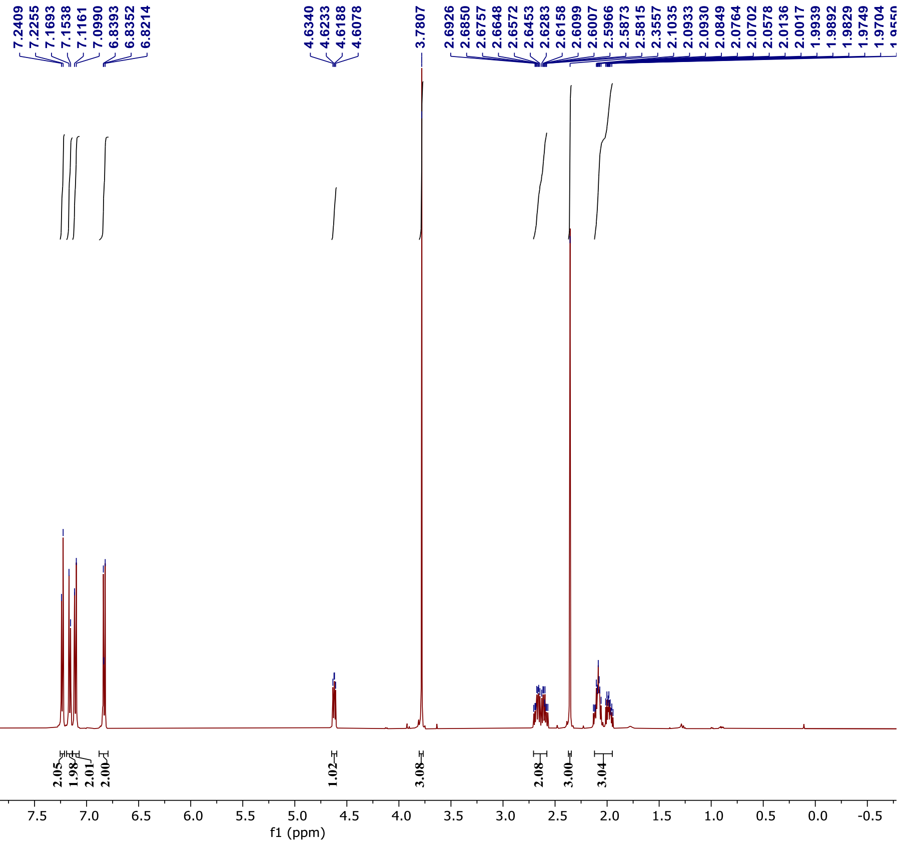

OH
NO2
¹³C{¹H} NMR (CDCl3, 125 MHz)
129.33 128.78 128.05 125.90 123.77
77.35 77.10 76.85 73.72
39.95
32.06
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

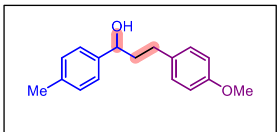

OH
OMe
¹H NMR (CDCl3, 500 MHz)
7.6651 7.6606 7.6485 7.6435 7.5464 7.3554 7.3470 7.3036 7.2993 7.2868 7.2828 7.2777 7.2410 7.1251 7.1020 7.0955
4.7165 4.7030 4.6895
3.8971
2.8872 2.8796 2.8699 2.8590 2.8514 2.8402 2.8260 2.8129 2.8072 2.7984 2.7943 2.7852 2.7796 2.7662 2.2091 2.2030 2.1982 2.1909 2.1803 2.1634 2.1289 2.1173 2.1099 2.1054 2.0992 2.0990 2.0871 2.0337 1.9334
2.06 0.98 3.85 1.98 2.02 1.00 3.03 2.10 1.04 1.12 0.81
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


OH
OMe
¹³C{¹H} NMR (CDCl3, 100MHz)
157.25 144.69 136.98 133.07 129.18 128.97 128.60 127.86 127.72 126.90 126.39 126.02 118.77
105.72
77.42 77.10 76.78
55.36
40.50
32.05
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

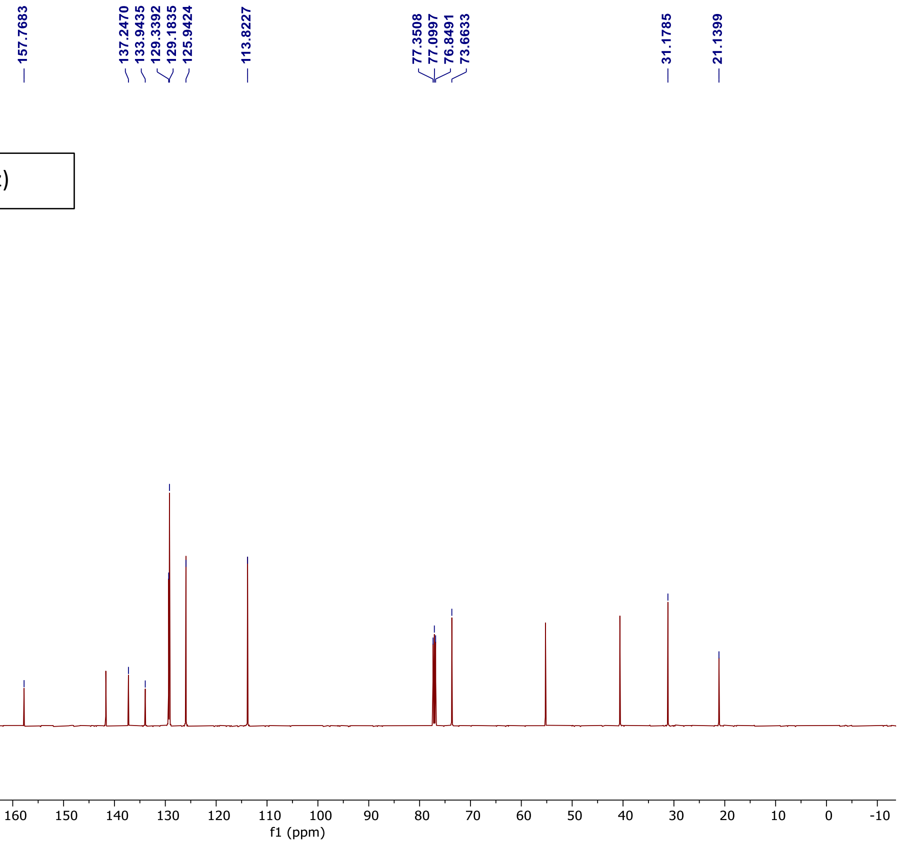


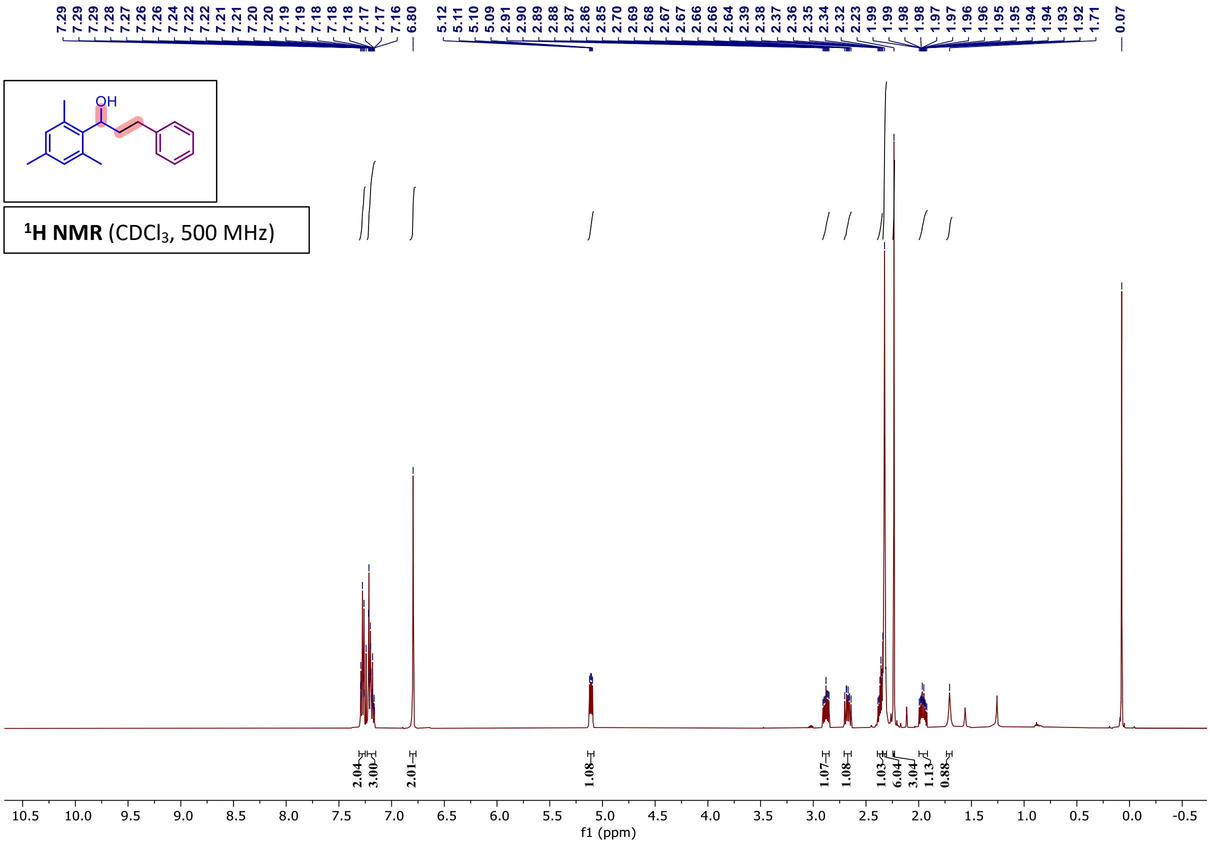
^{1}H NMR ($CDCl_3$, 500 MHz)

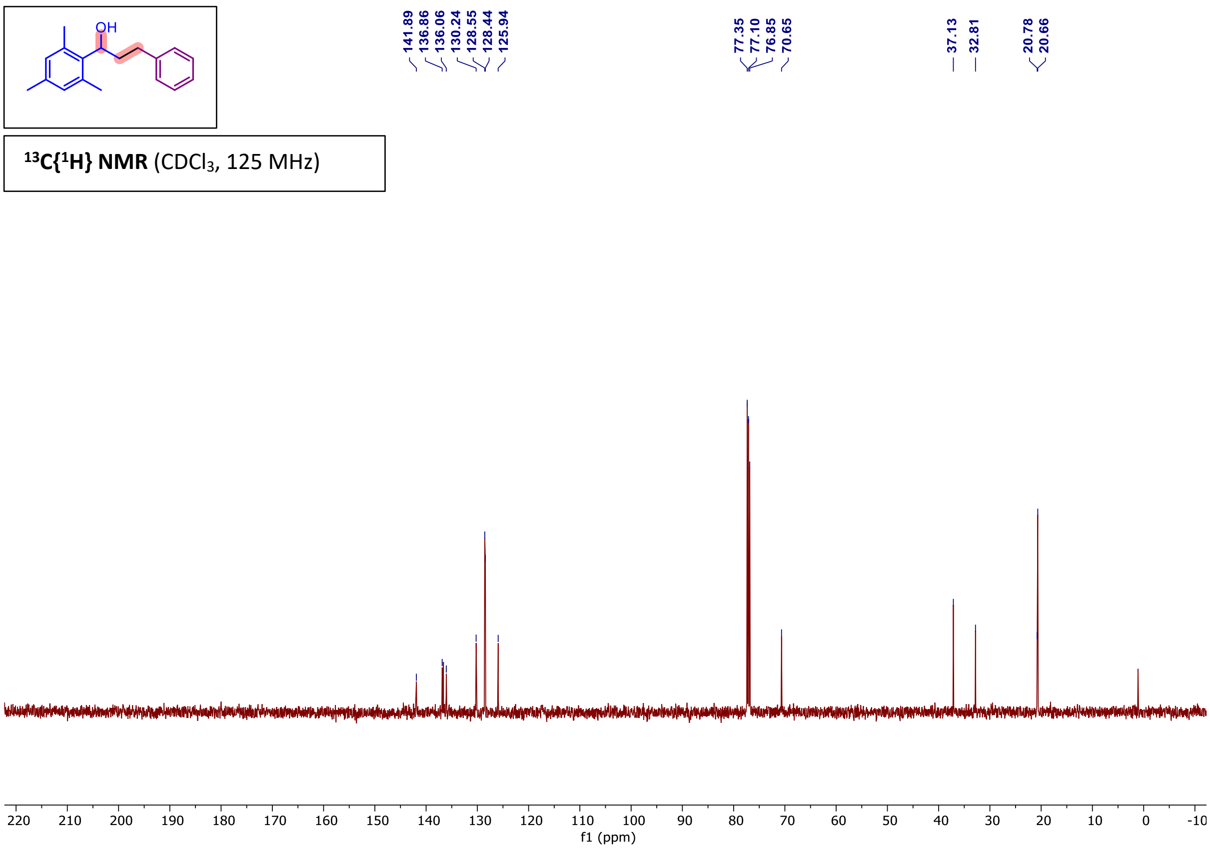


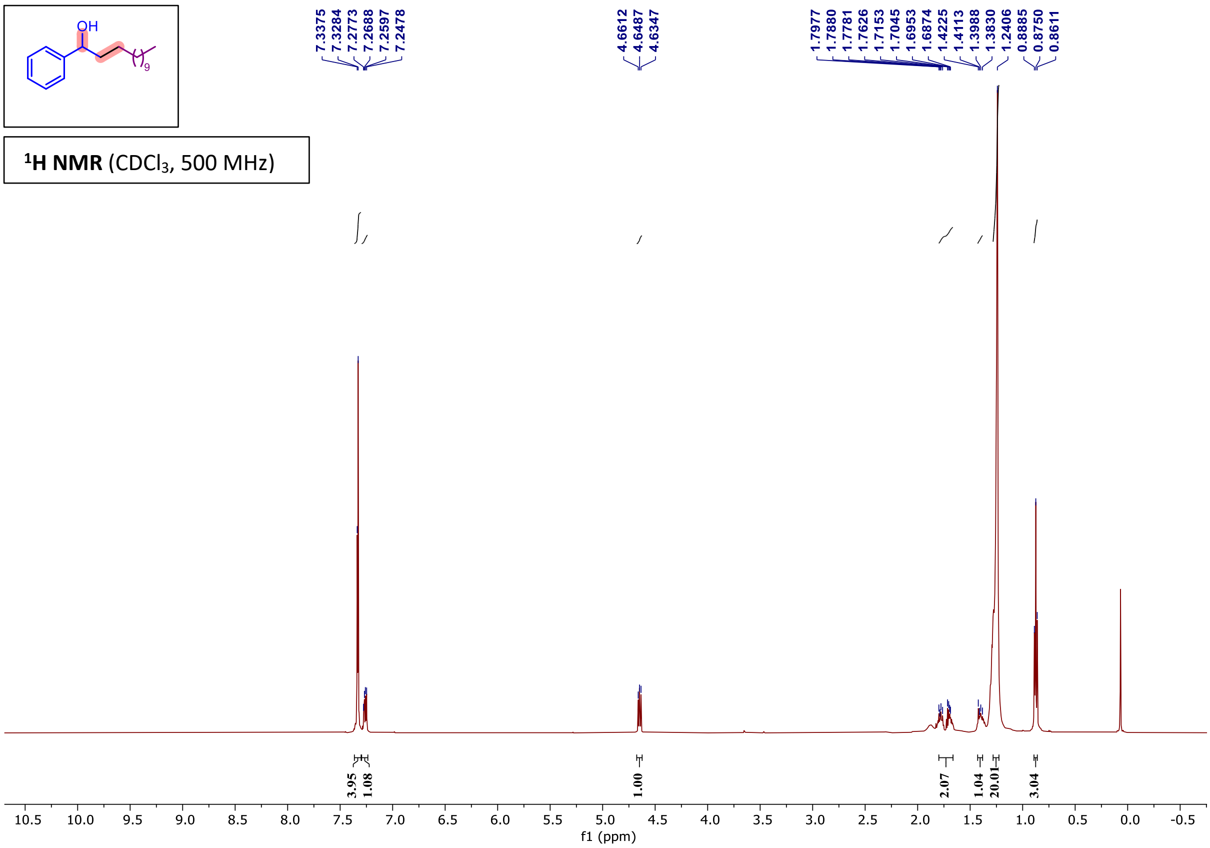


^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)

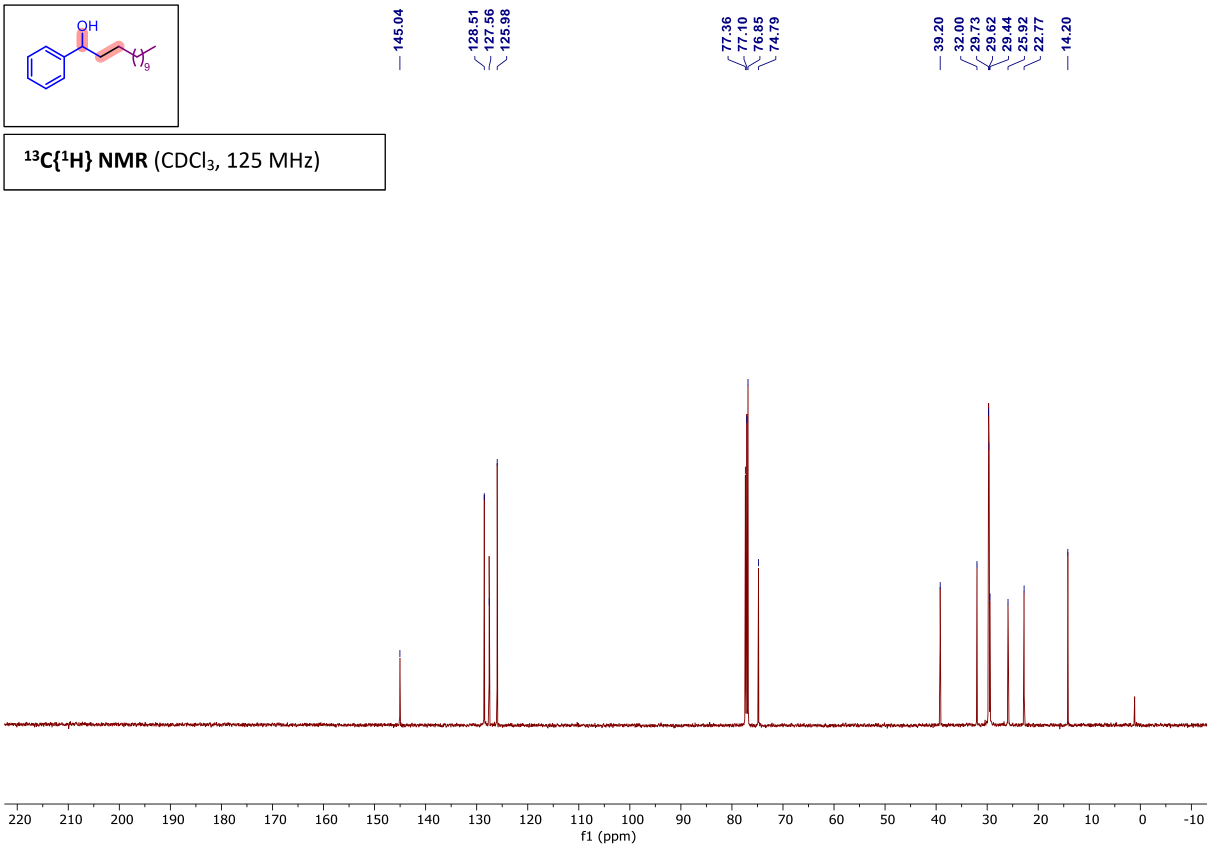



OH
¹H NMR (CDCl₃, 500 MHz)
f1 (ppm)

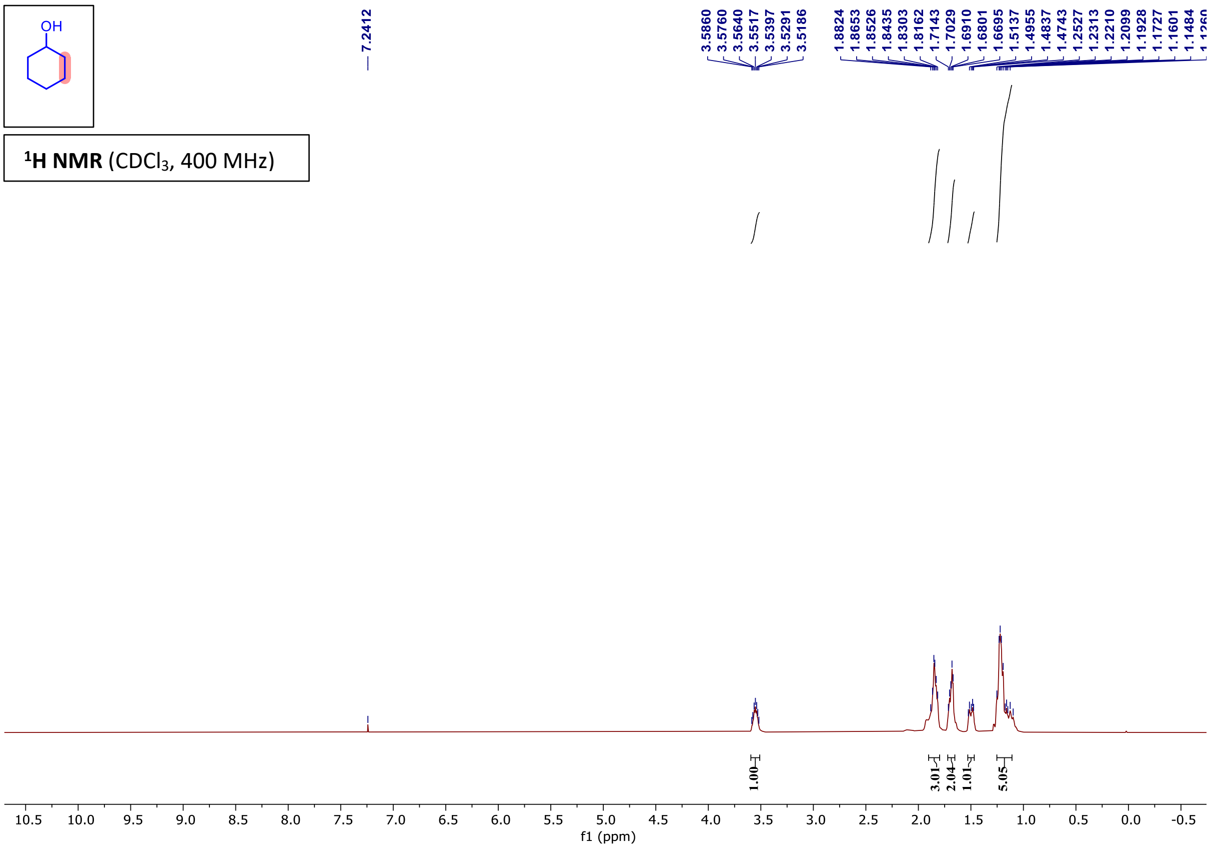

OH
¹³C{¹H} NMR (CDCl₃, 125 MHz)
f1 (ppm)

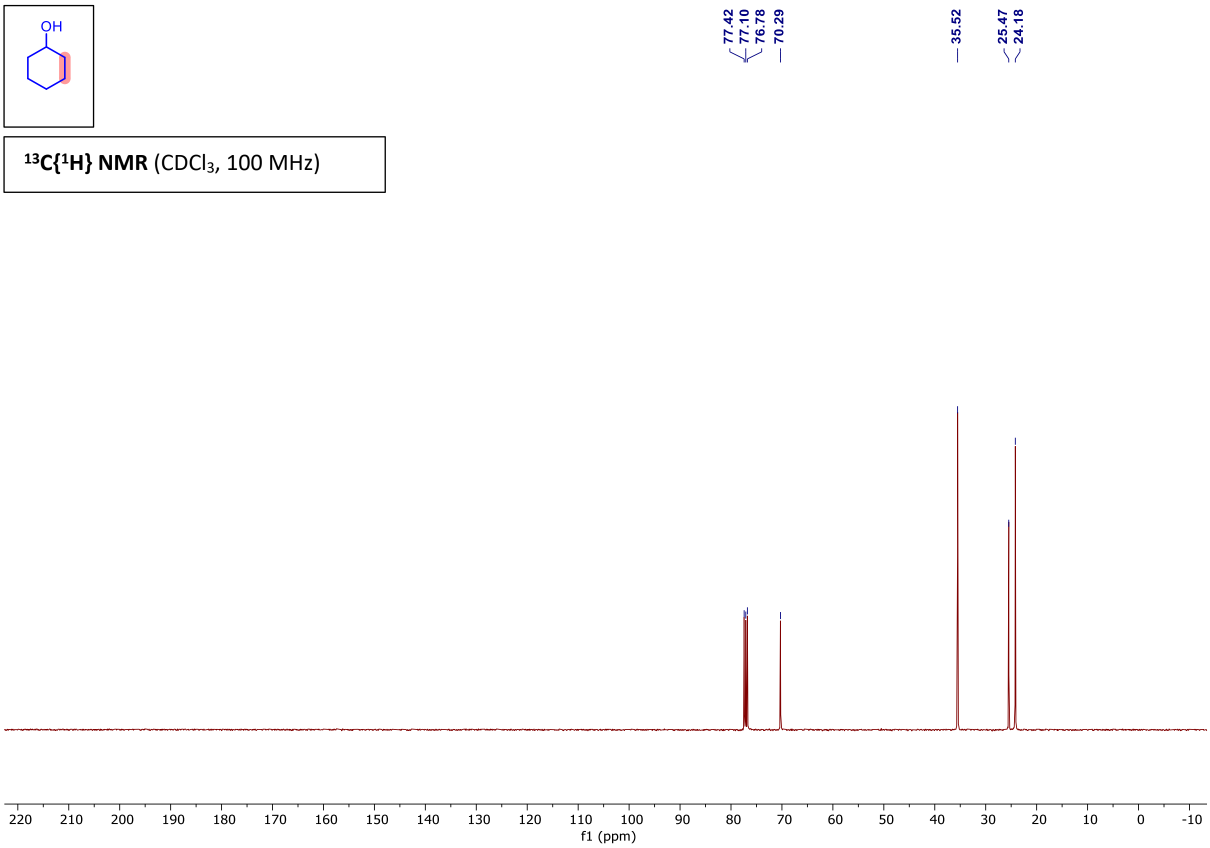


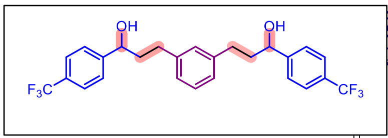
[1]H NMR (CDCl$_3$, 500 MHz)



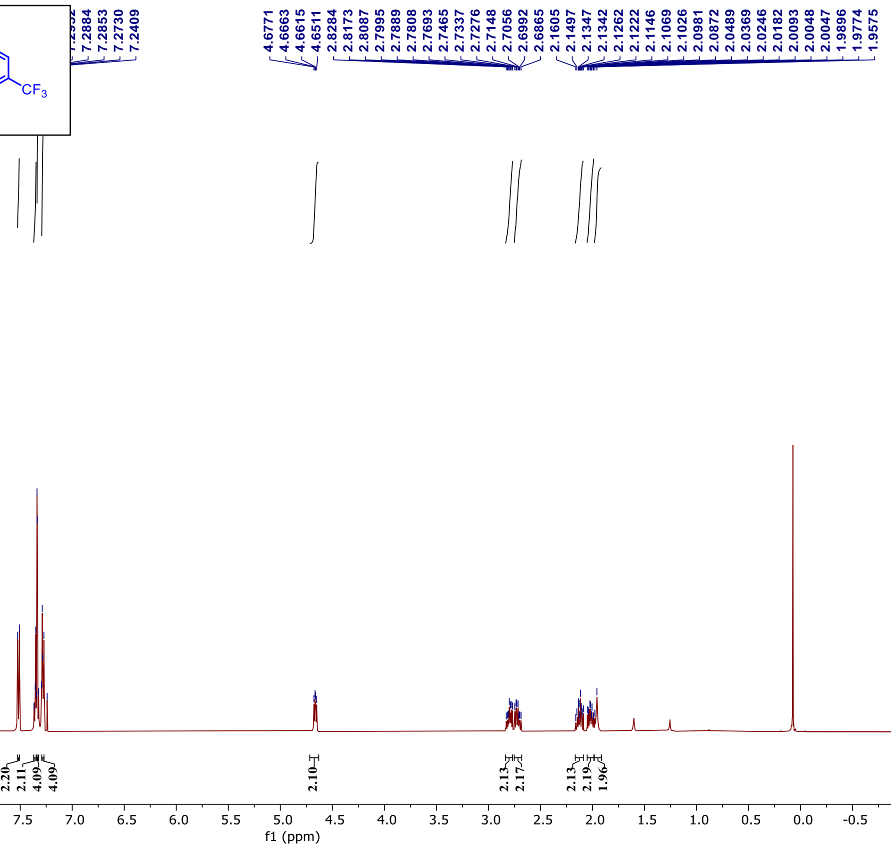
[13]C{[1]H} NMR (CDCl$_3$, 125 MHz)

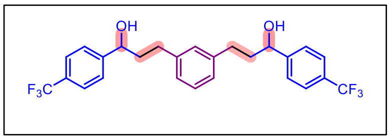

OH
¹H NMR ($CDCl_3$, 400 MHz)
7.2412
3.5860 3.5760 3.5640 3.5517 3.5397 3.5291 3.5186
1.8824 1.8653 1.8526 1.8435 1.8303 1.8162 1.7143 1.7029 1.6910 1.6801 1.6695 1.5137 1.4955 1.4837 1.4743 1.2527 1.2313 1.2210 1.2099 1.1928 1.1727 1.1601 1.1484
1.00
3.01
2.04
1.01
5.05
f1 (ppm)


OH
¹³C{¹H} NMR ($CDCl_3$, 100 MHz)
77.42
77.10
76.78
70.29
35.52
25.47
24.18
f1 (ppm)

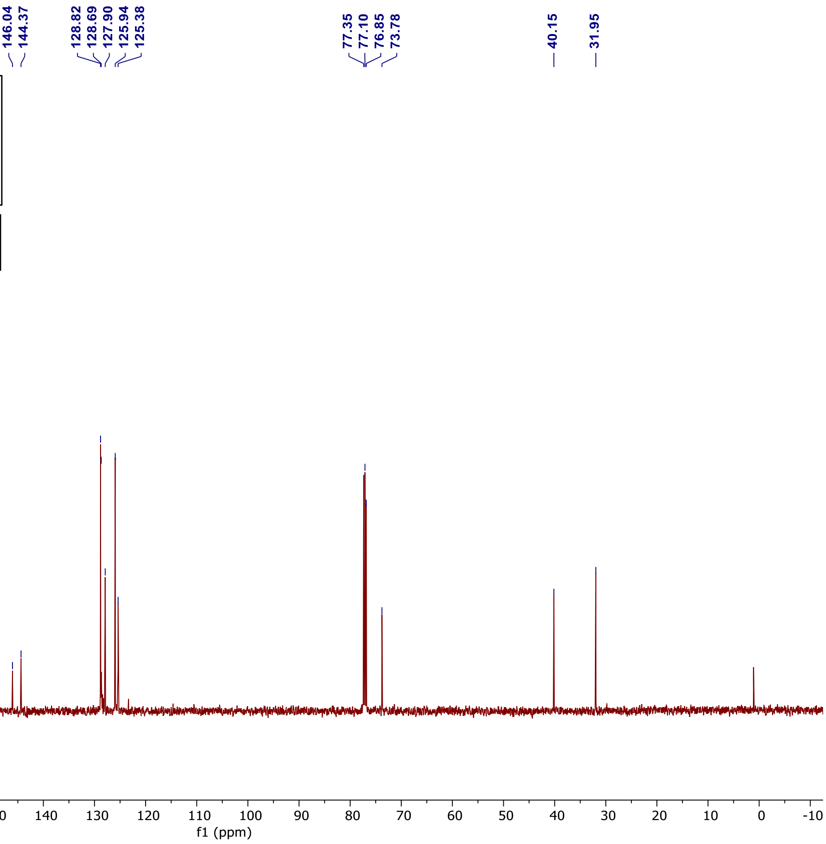


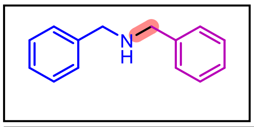
^{1}H NMR ($CDCl_3$, 500 MHz)



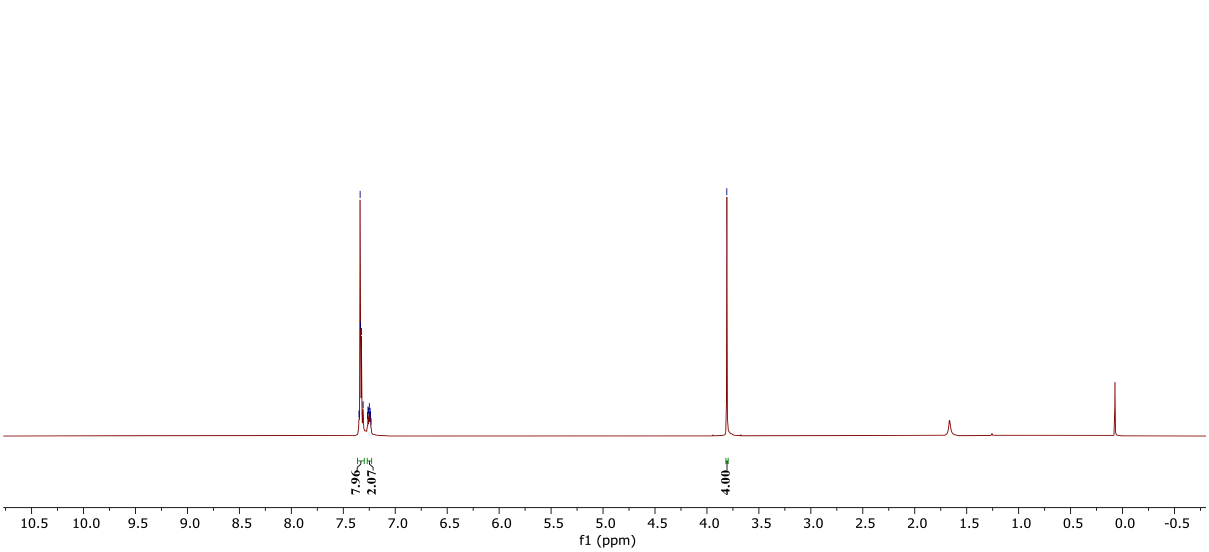


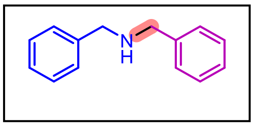
$^{13}C\{^1H\}$ NMR ($CDCl_3$, 125 MHz)



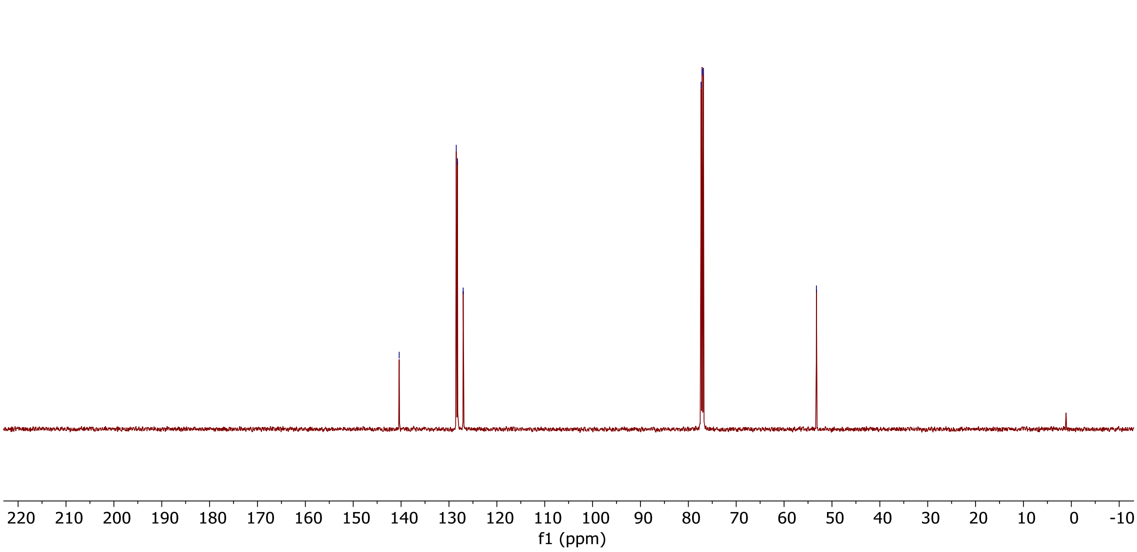


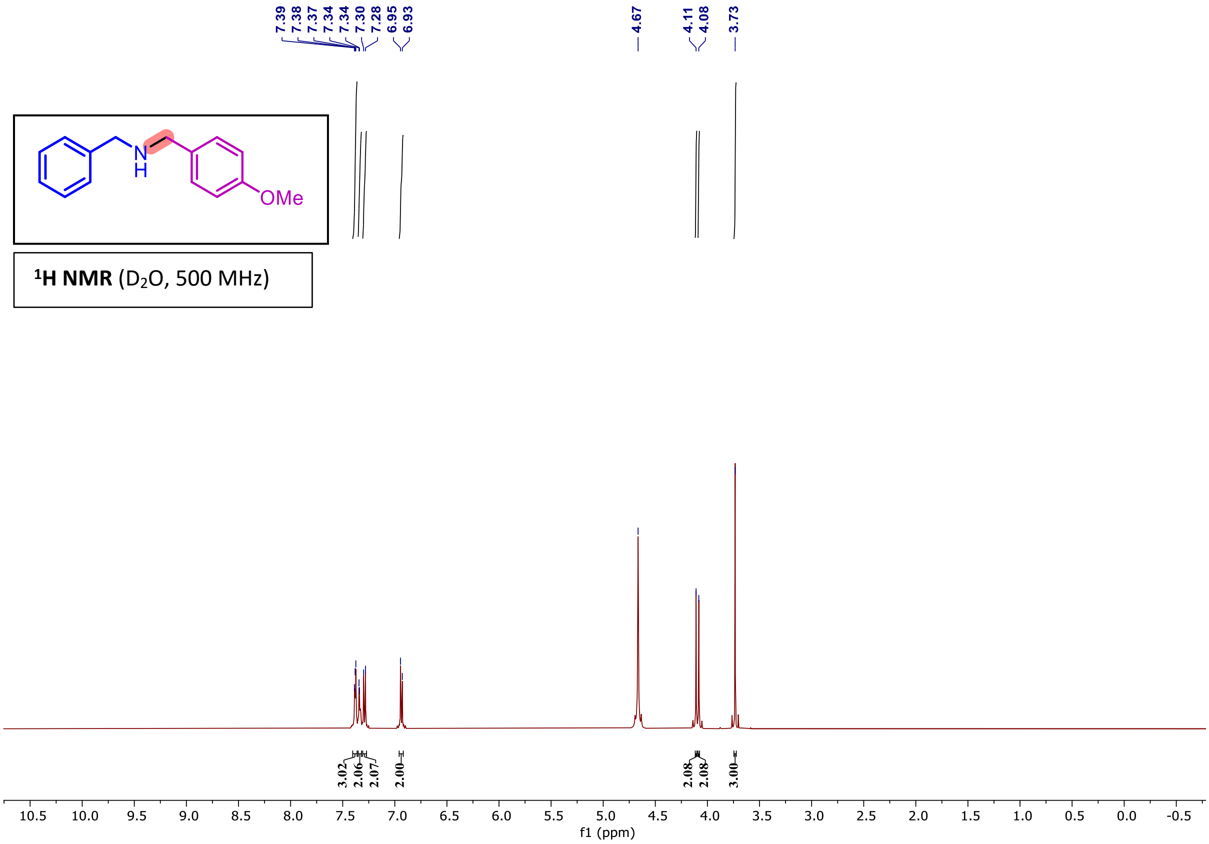
¹H NMR ($CDCl_3$, 500 MHz)



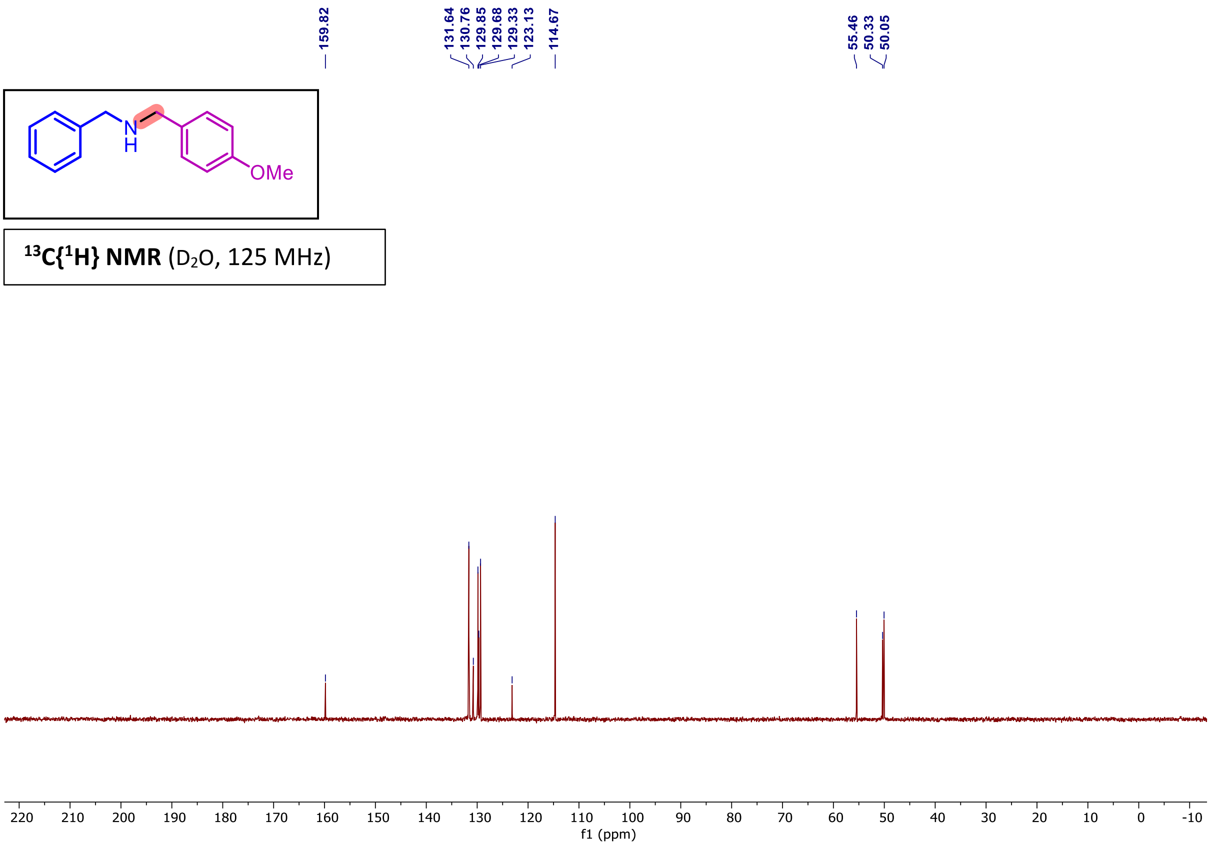


¹³C{¹H} NMR ($CDCl_3$, 125 MHz)

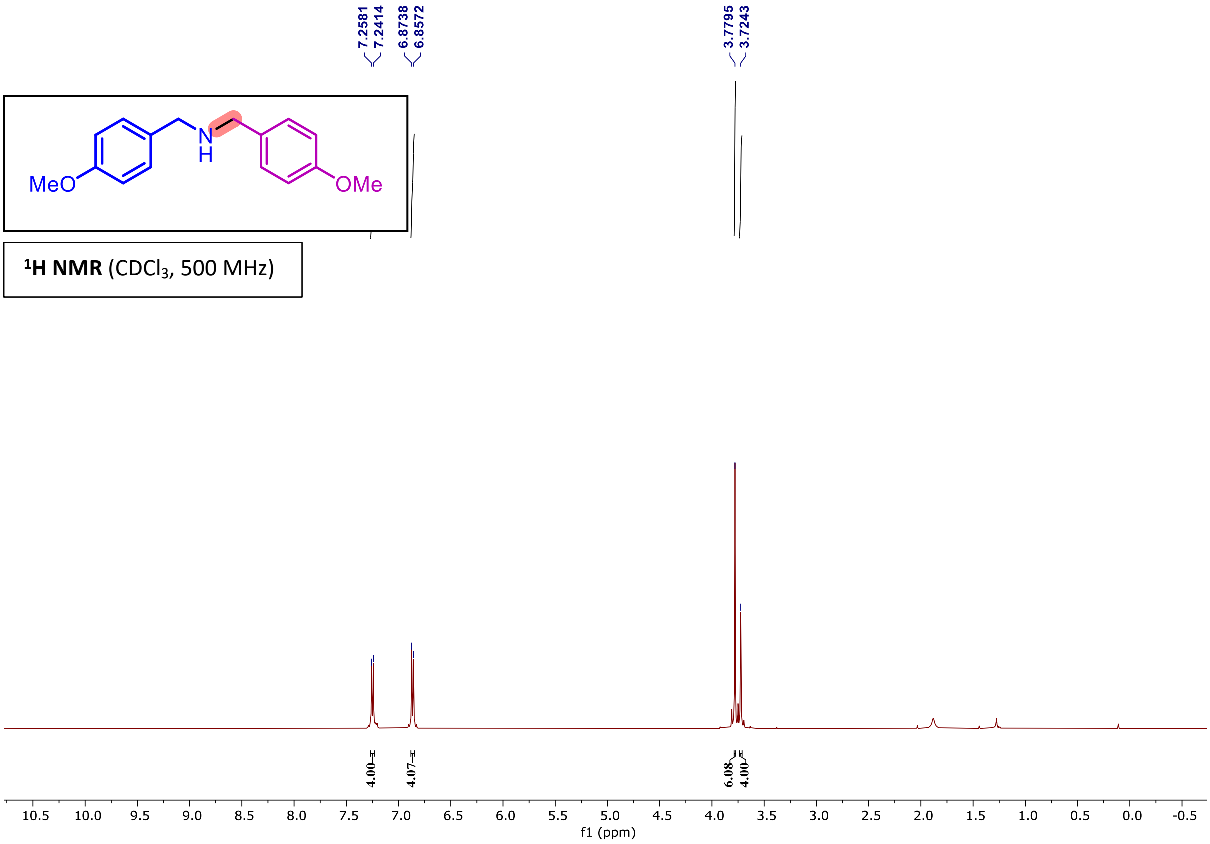


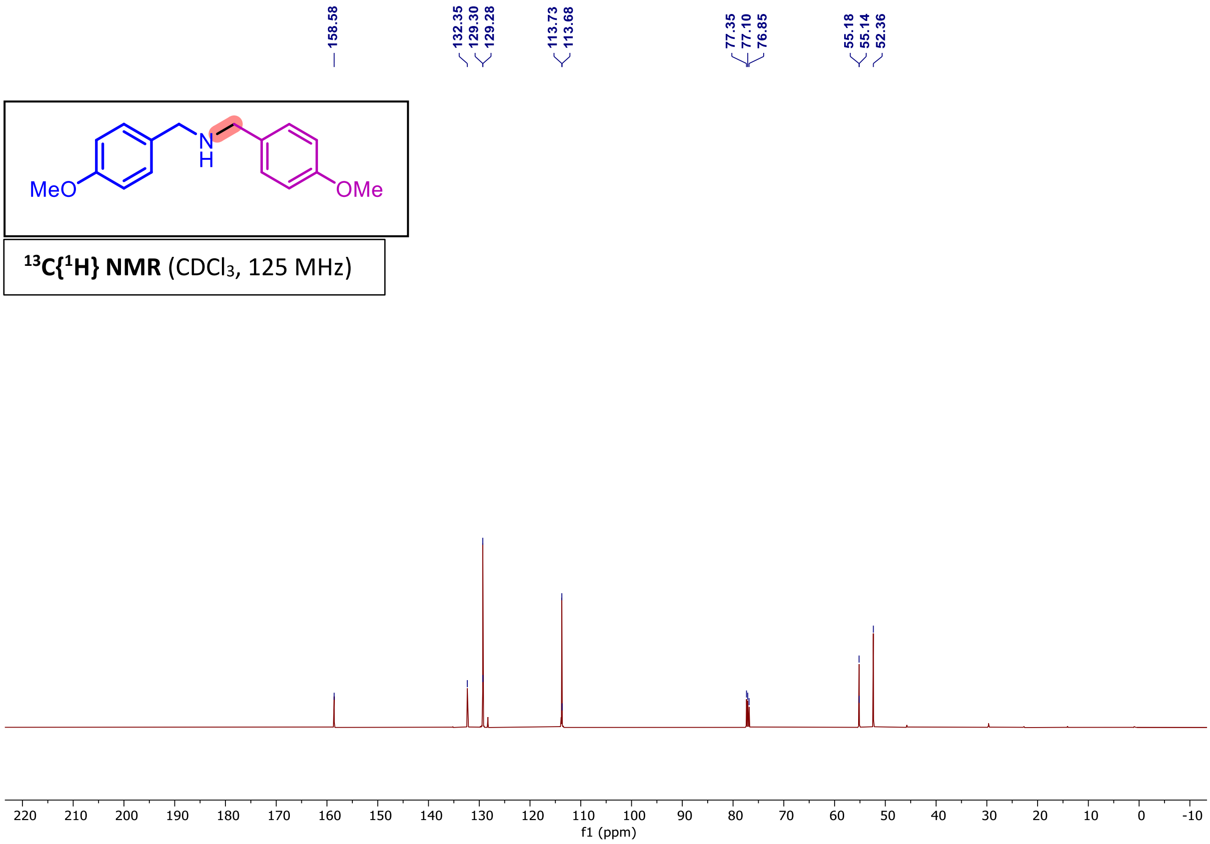


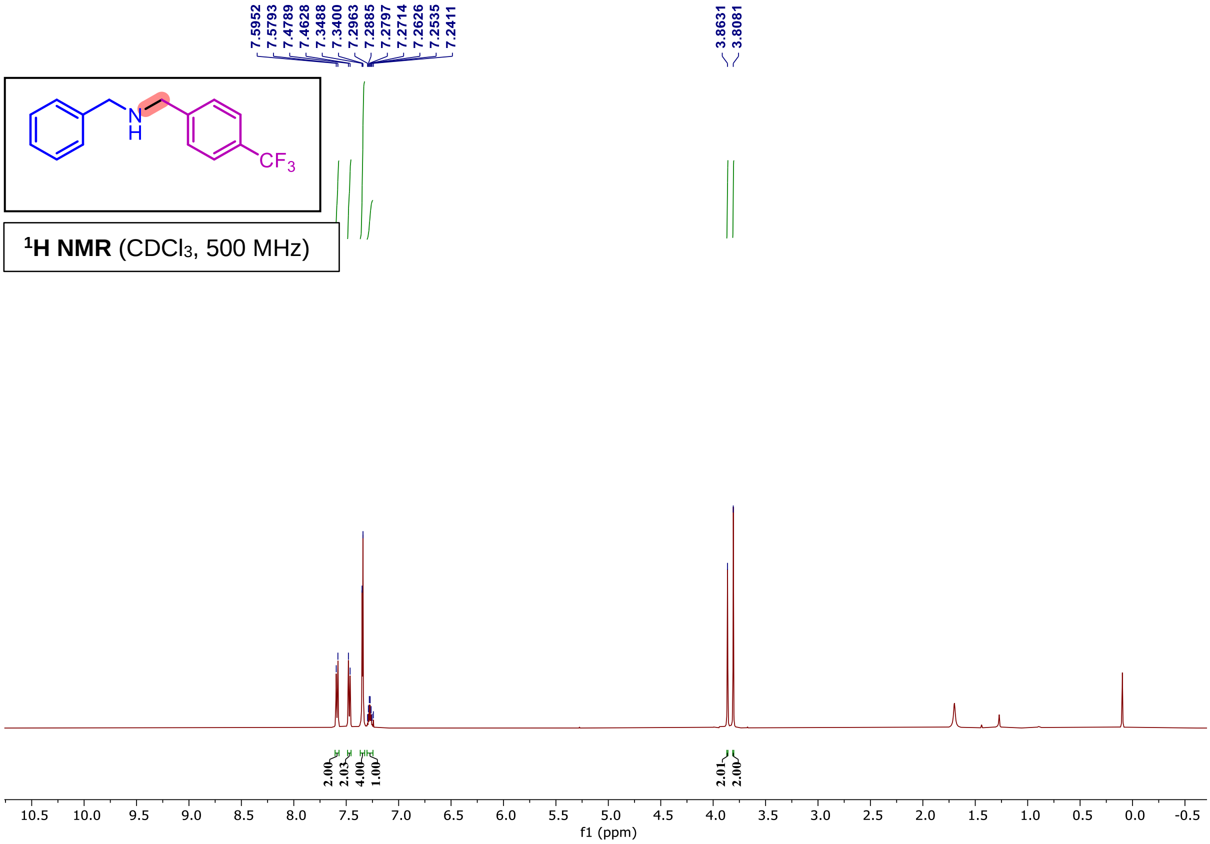
^{1}H NMR (D_2O, 500 MHz)

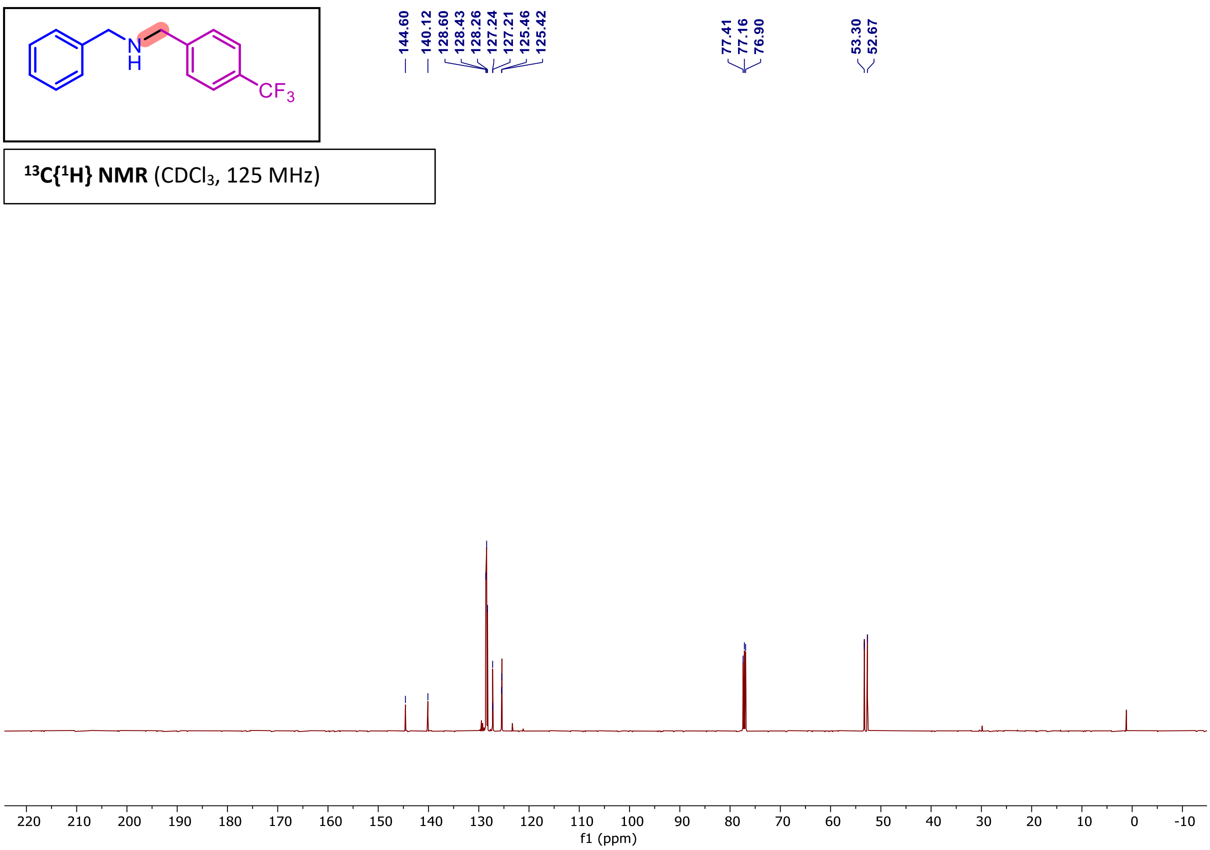


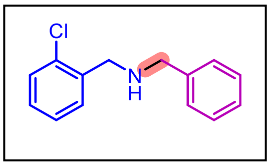
^{13}C{^{1}H} NMR (D_2O, 125 MHz)


7.2581
7.2414
6.8738
6.8572
3.7795
3.7243
MeO
N
H
OMe
1H NMR (CDCl3, 500 MHz)
4.00
4.07
6.08
4.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

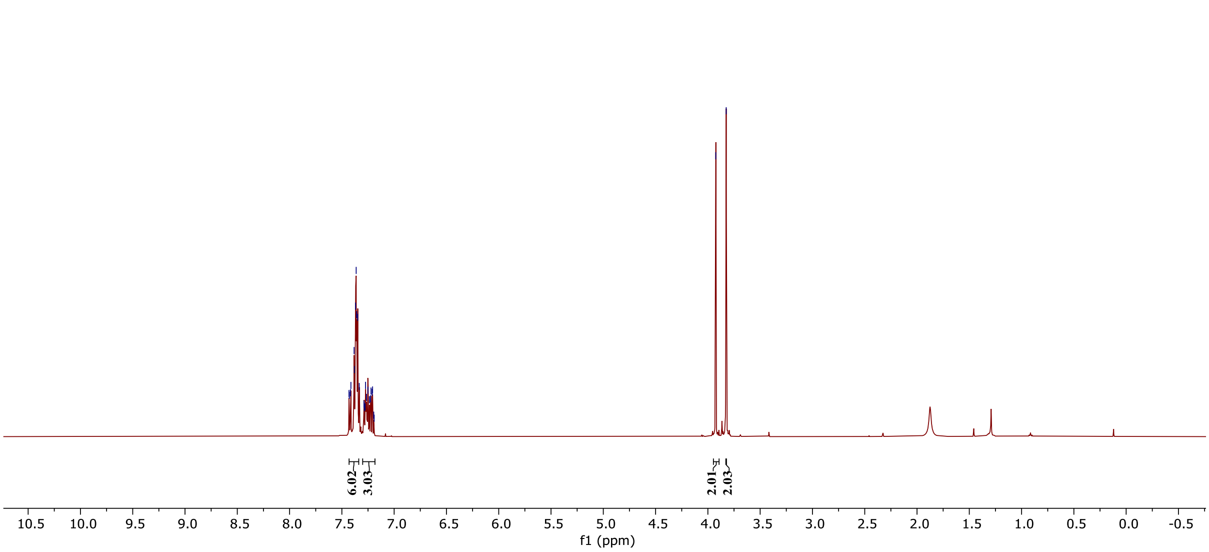

158.58
132.35
129.30
129.28
113.73
113.68
77.35
77.10
76.85
55.18
55.14
52.36
MeO
N
H
OMe
13C{1H} NMR (CDCl3, 125 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

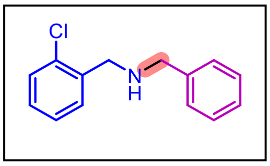

7.5952
7.5793
7.4789
7.4628
7.3488
7.3400
7.2963
7.2885
7.2797
7.2714
7.2626
7.2535
7.2411
3.8631
3.8081
N
H
CF3
1H NMR (CDCl3, 500 MHz)
2.00
2.03
4.00
1.00
2.01
2.00
f1 (ppm)


144.60
140.12
128.60
128.43
128.26
127.24
127.21
125.46
125.42
77.41
77.16
76.90
53.30
52.67
N
H
CF3
13C{1H} NMR (CDCl3, 125 MHz)
f1 (ppm)

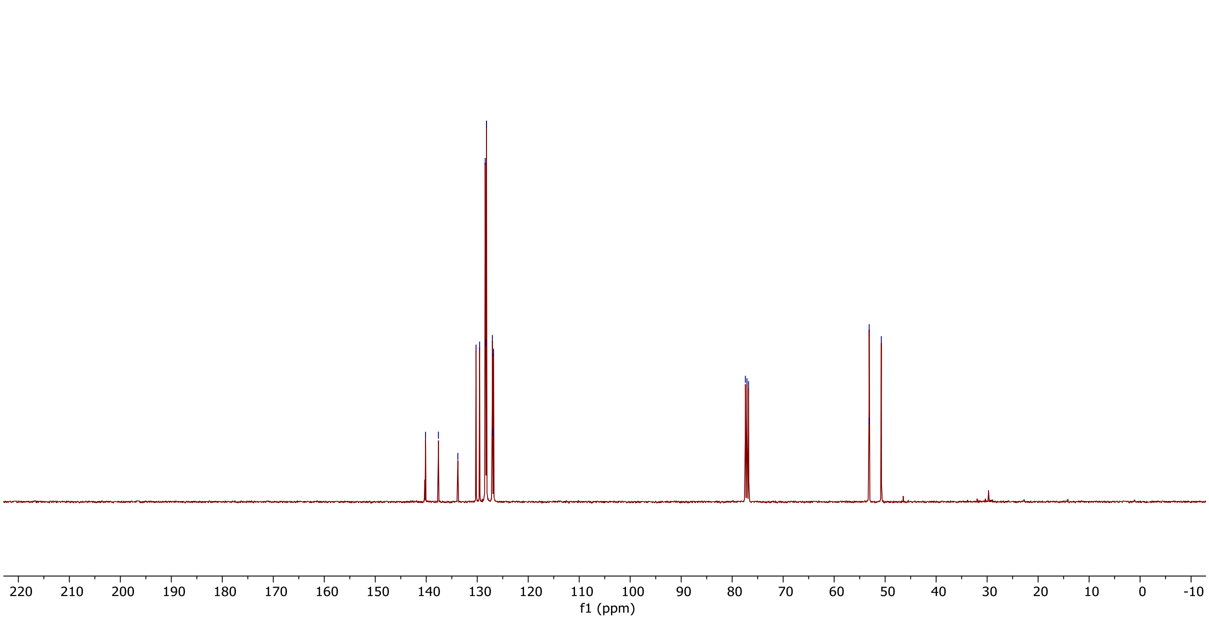


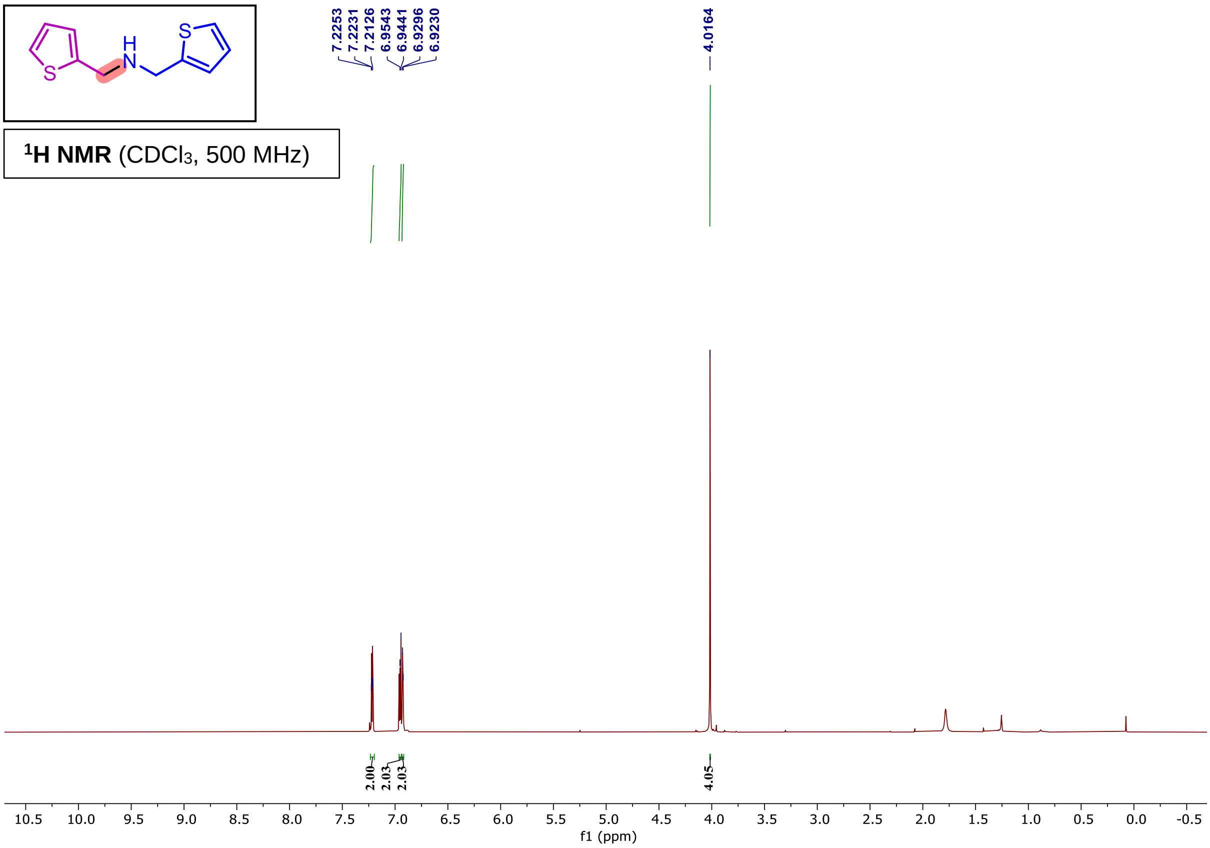
¹H NMR ($CDCl_3$, 500 MHz)



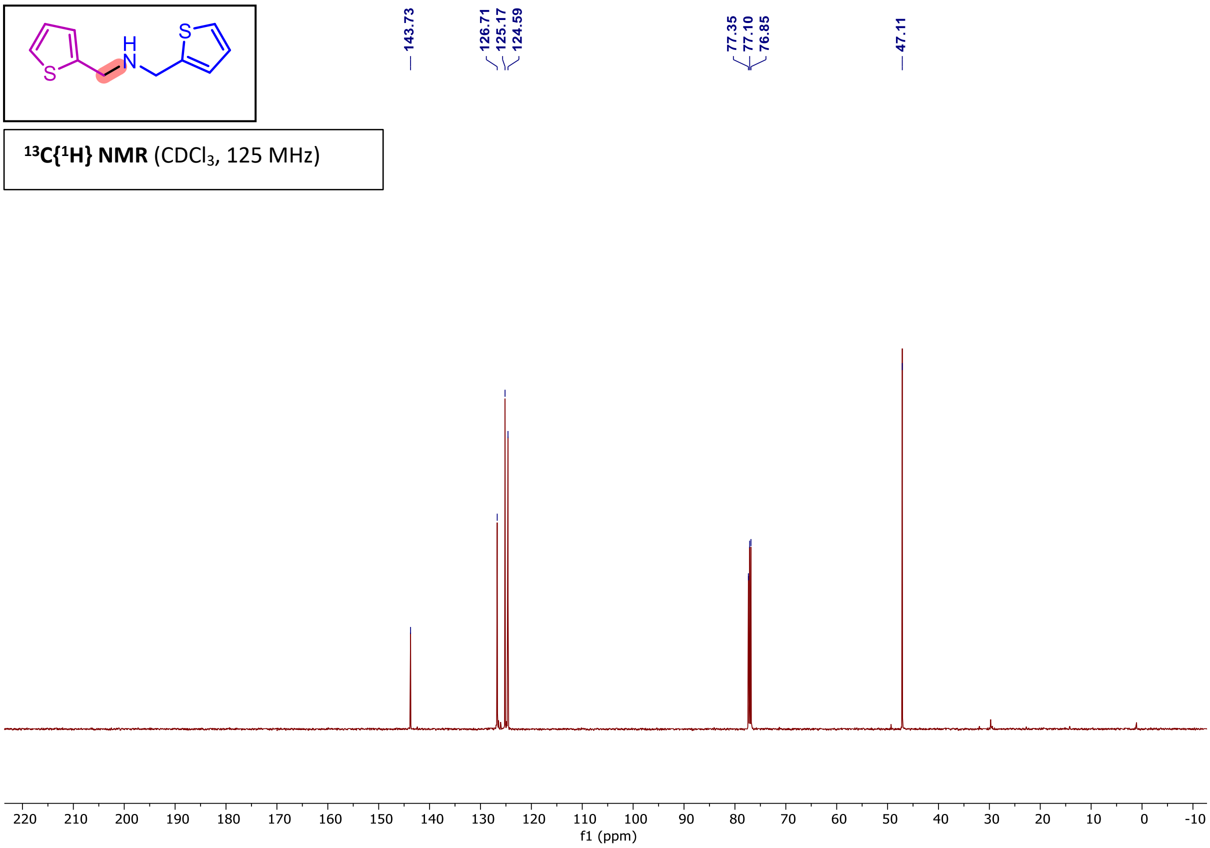


¹³C{¹H} NMR ($CDCl_3$, 100 MHz)

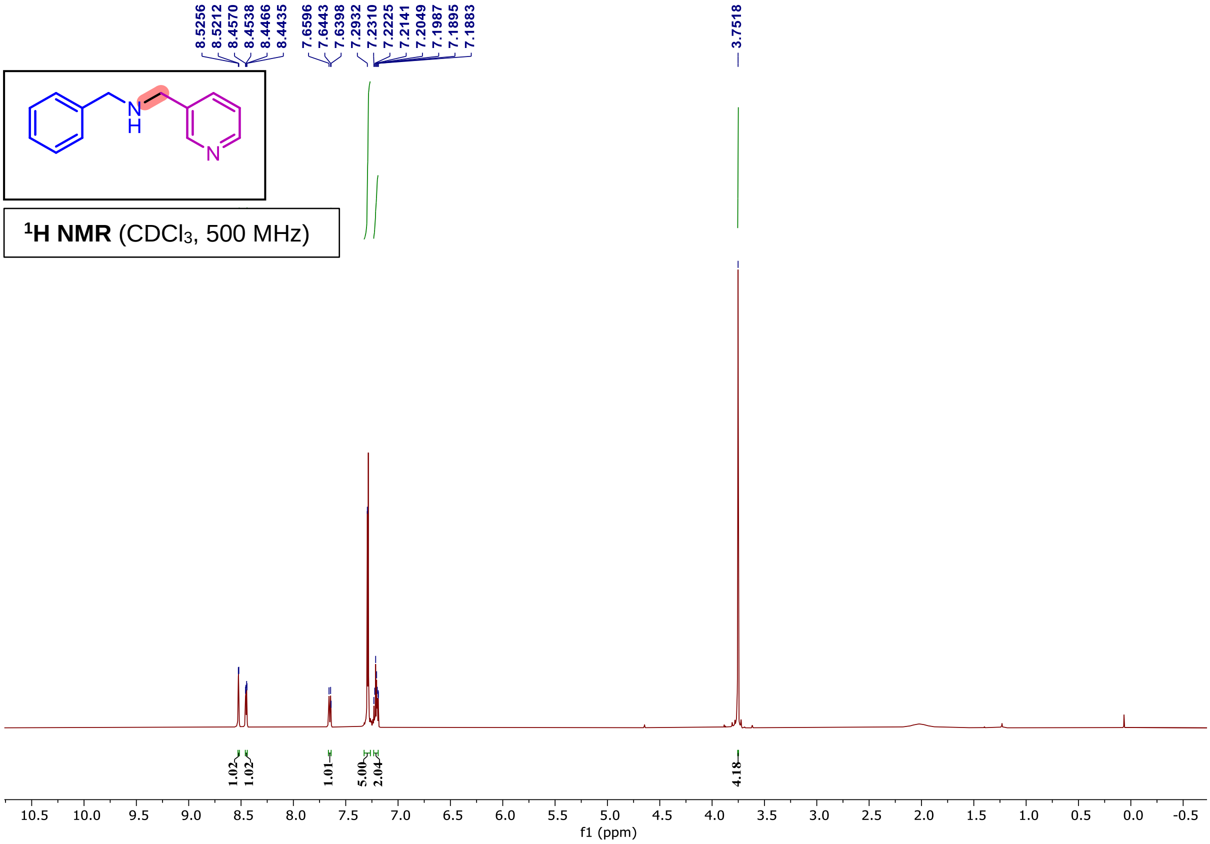




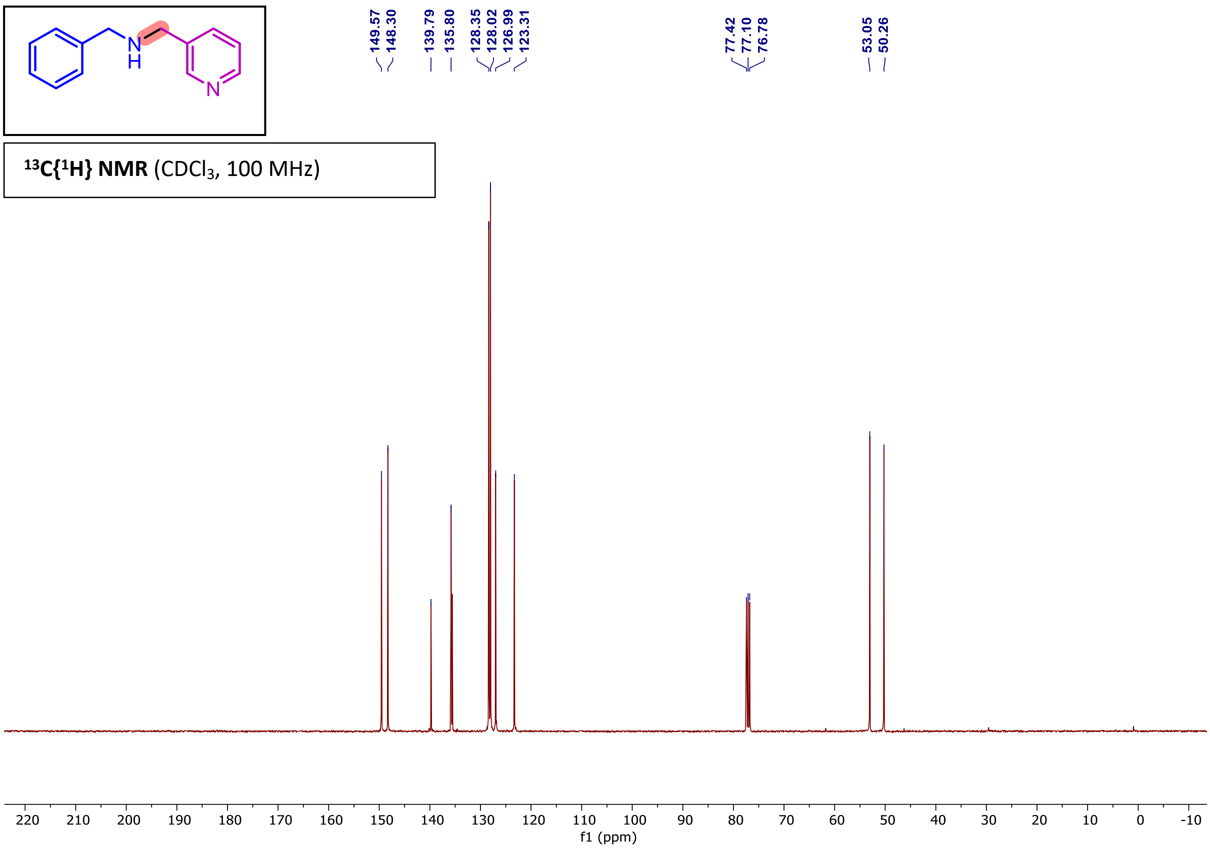
¹H NMR (CDCl3, 500 MHz)
7.2253
7.2231
7.2126
6.9543
6.9441
6.9296
6.9230
4.0164
2.00
2.03
2.03
4.05
f1 (ppm)



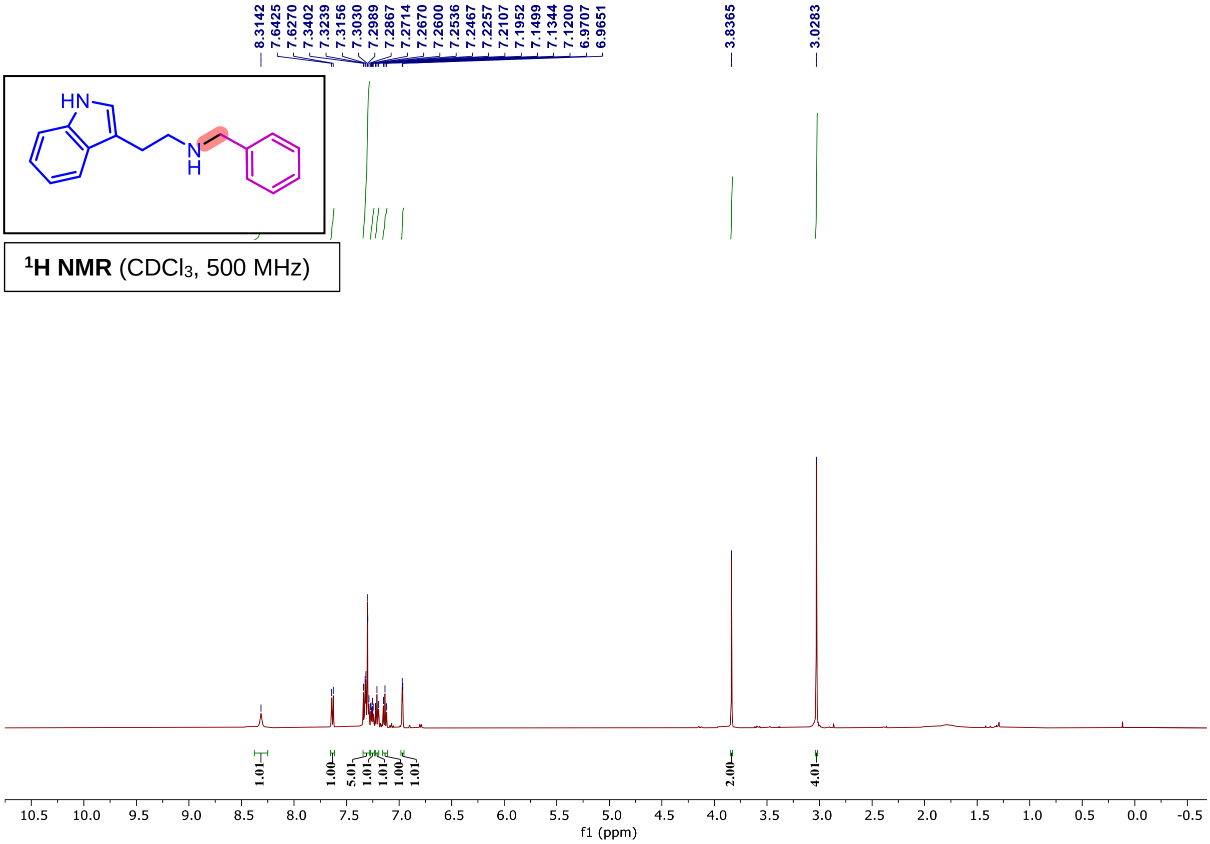
¹³C{¹H} NMR (CDCl3, 125 MHz)
143.73
126.71
125.17
124.59
77.35
77.10
76.85
47.11
f1 (ppm)

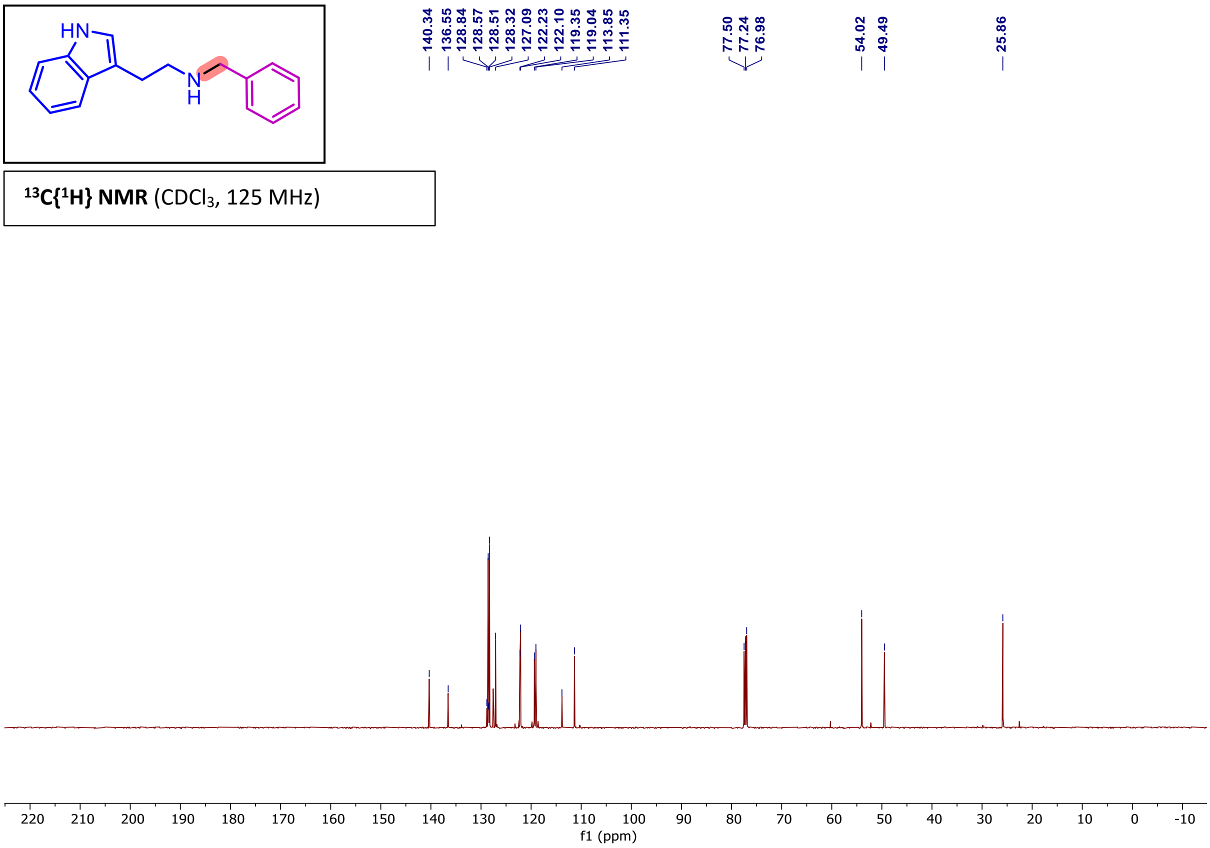


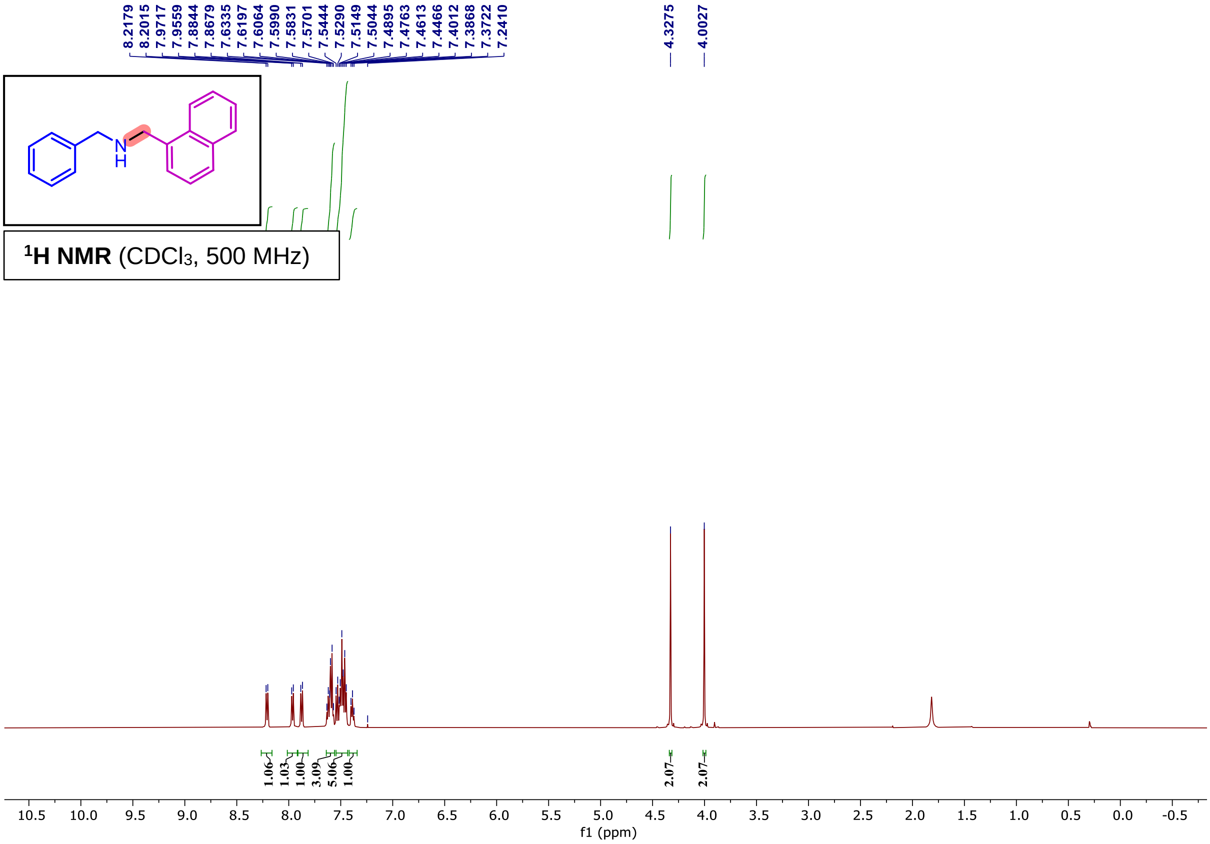
N
H
N
¹H NMR (CDCl₃, 500 MHz)
f1 (ppm)



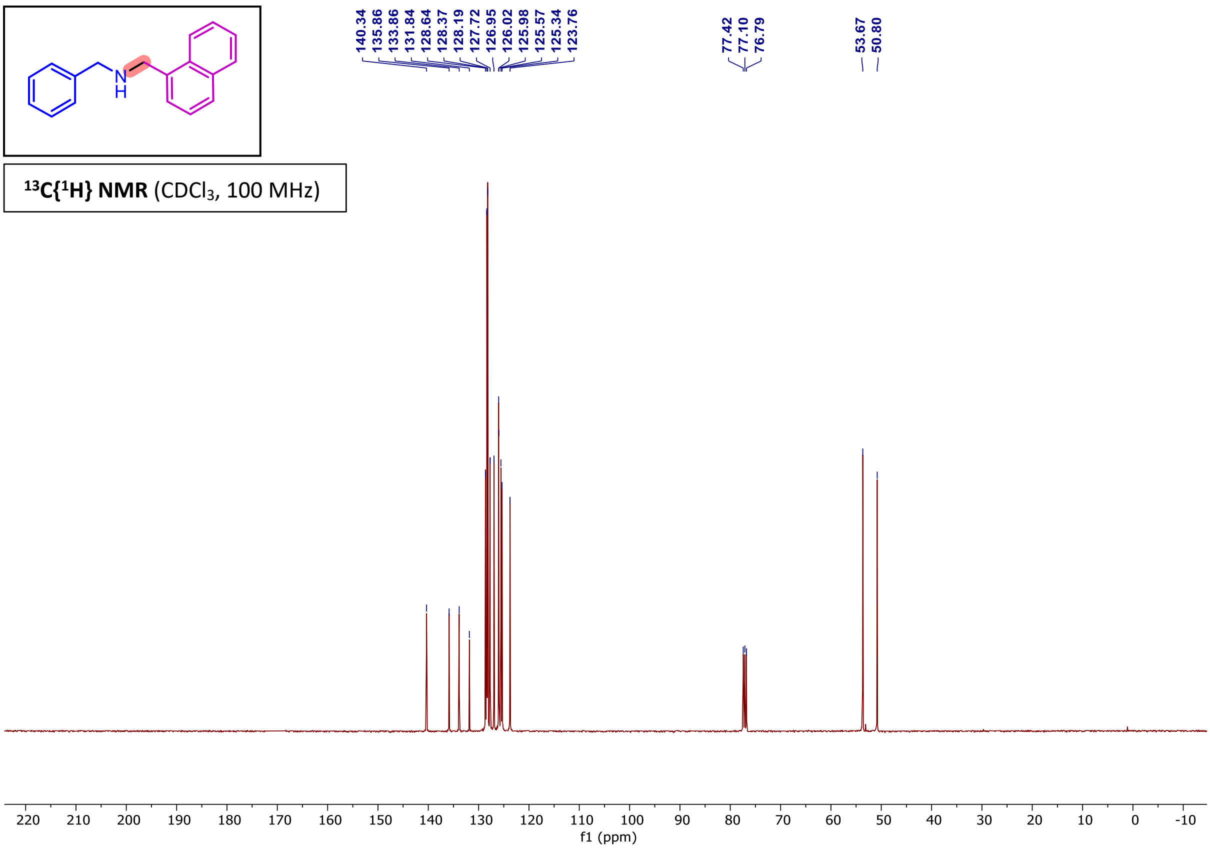
N
H
N
¹³C{¹H} NMR (CDCl₃, 100 MHz)
f1 (ppm)


HN
N
H
¹H NMR (CDCl₃, 500 MHz)
8.3142
7.6425
7.6270
7.3402
7.3239
7.3156
7.3030
7.2989
7.2867
7.2714
7.2670
7.2600
7.2536
7.2467
7.2257
7.2107
7.1952
7.1499
7.1344
7.1200
6.9707
6.9651
3.8365
3.0283
1.01
1.00
5.01
1.01
1.01
1.00
1.01
2.00
4.01
f1 (ppm)

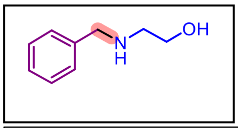

HN
N
H
¹³C{¹H} NMR (CDCl₃, 125 MHz)
140.34
136.55
128.84
128.57
128.51
128.32
127.09
122.23
122.10
119.35
119.04
113.85
111.35
77.50
77.24
76.98
54.02
49.49
25.86
f1 (ppm)



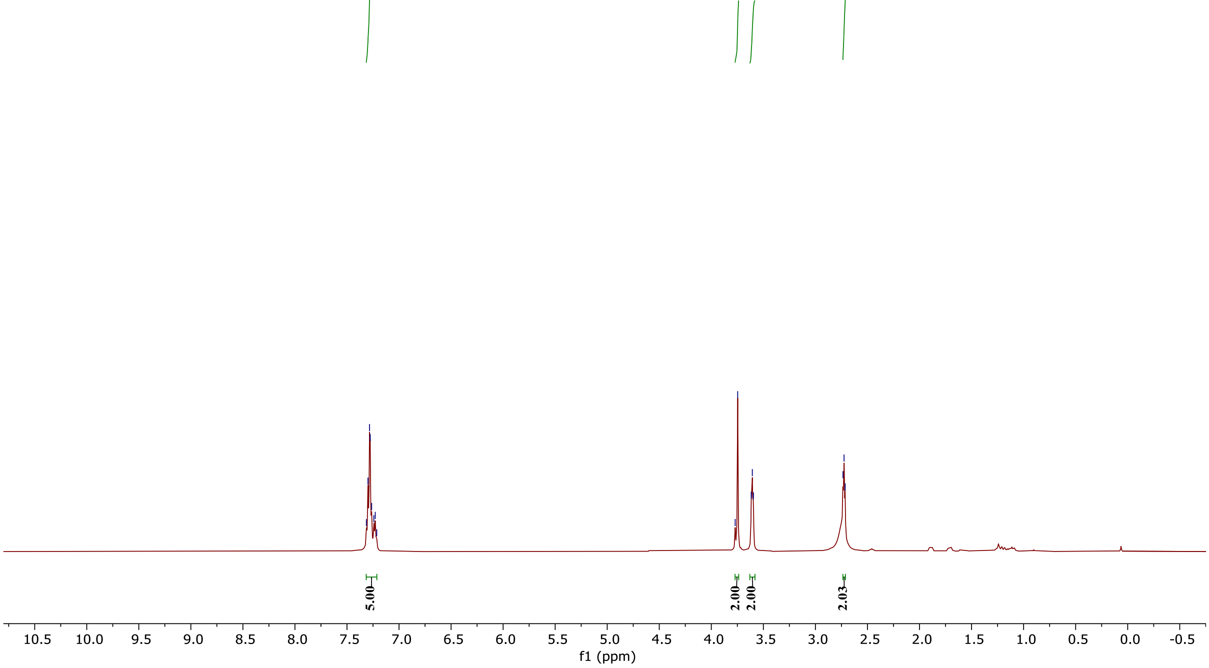
8.2179
8.2015
7.9717
7.9559
7.8844
7.8679
7.6335
7.6197
7.6064
7.5990
7.5831
7.5701
7.5444
7.5290
7.5149
7.5044
7.4895
7.4763
7.4613
7.4466
7.4012
7.3868
7.3722
7.2410
4.3275
4.0027
N
H
¹H NMR (CDCl₃, 500 MHz)
1.06
1.03
1.00
3.09
5.06
1.00
2.07
2.07
f1 (ppm)

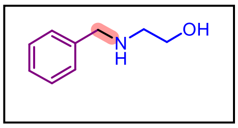


140.34
135.86
133.86
131.84
128.64
128.37
128.19
127.72
126.95
126.02
125.98
125.57
125.34
123.76
77.42
77.10
76.79
53.67
50.80
N
H
¹³C{¹H} NMR (CDCl₃, 100 MHz)
f1 (ppm)

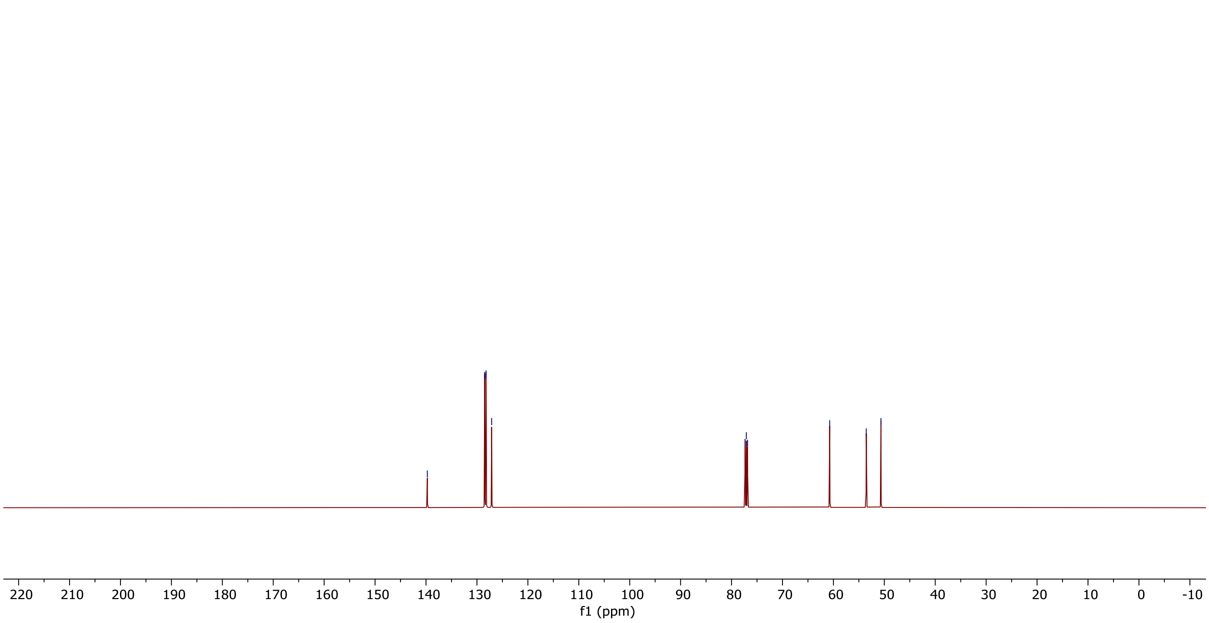


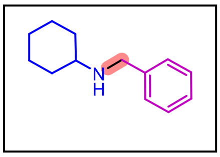
[1]H NMR ($CDCl_3$, 500 MHz)



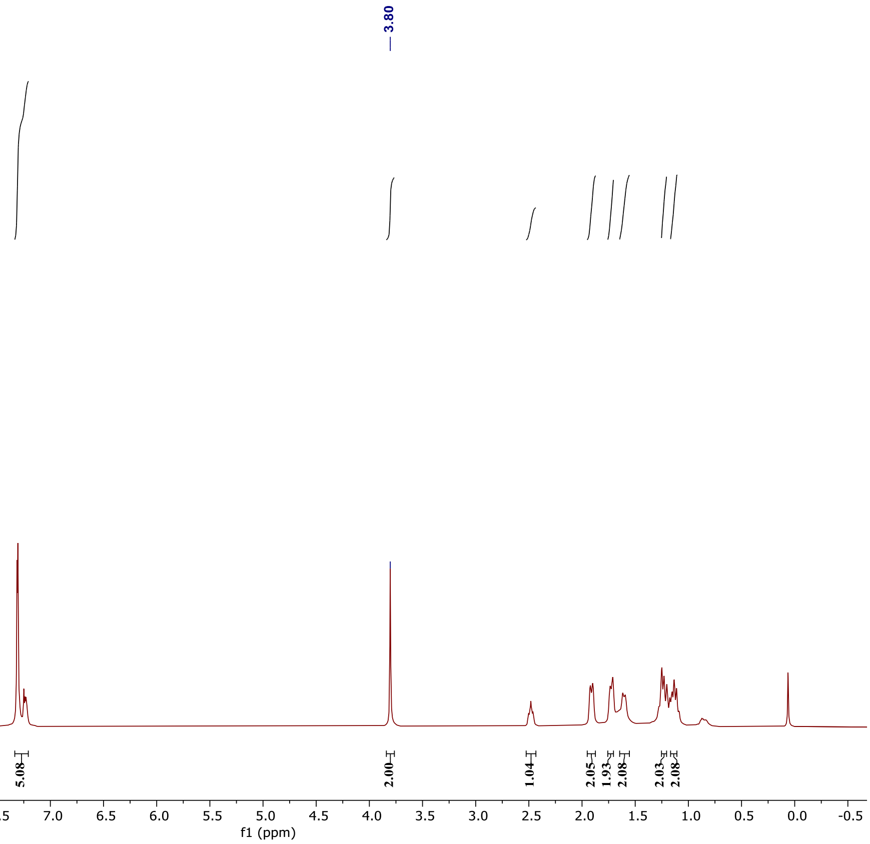


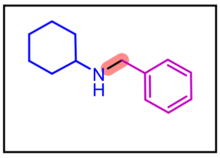
[13]C{[1]H} NMR ($CDCl_3$, 125 MHz)



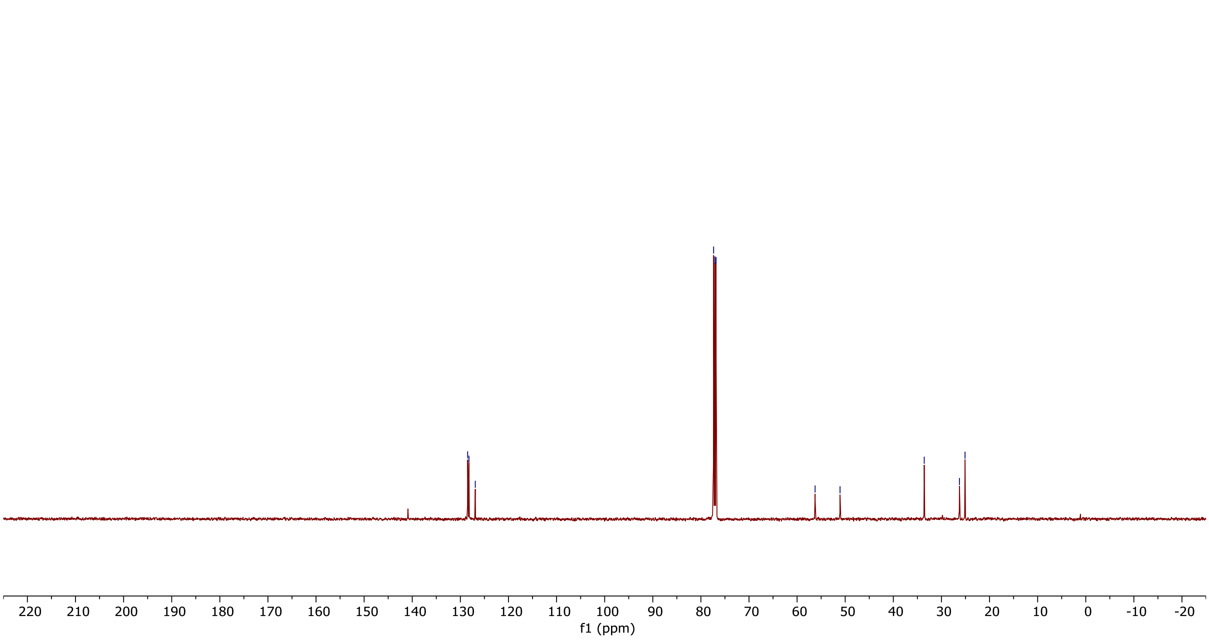


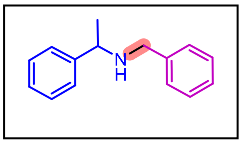
^{1}H NMR ($CDCl_3$, 500 MHz)



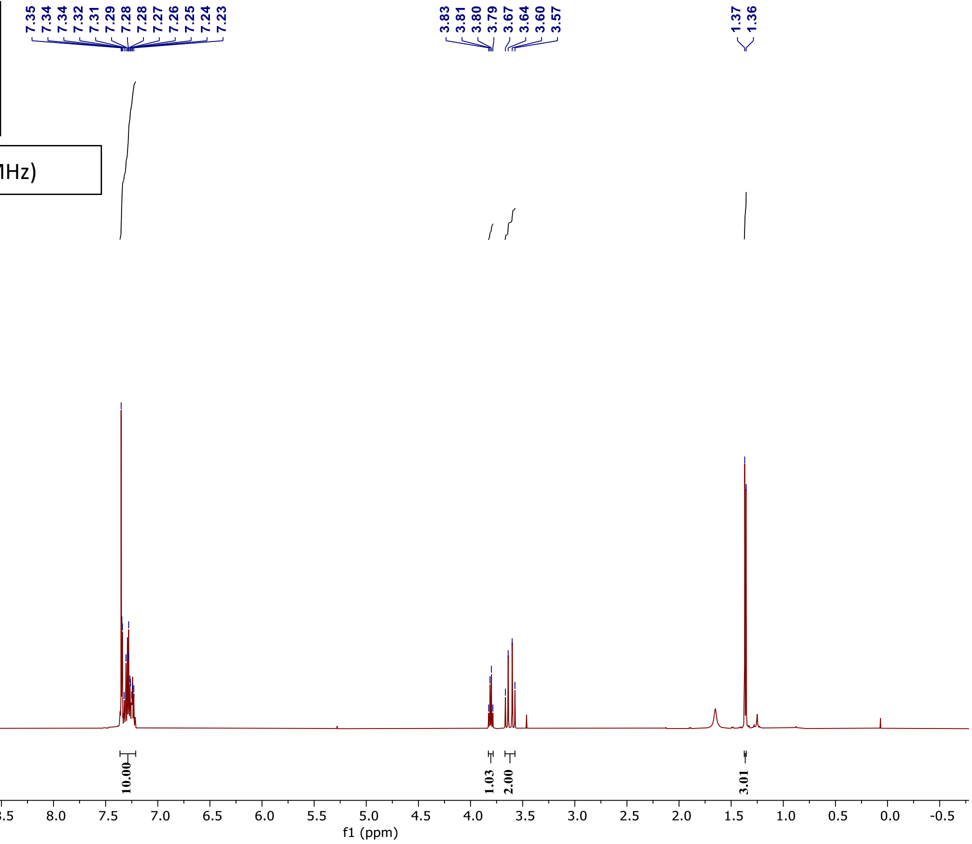


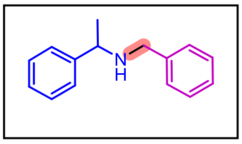
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz)



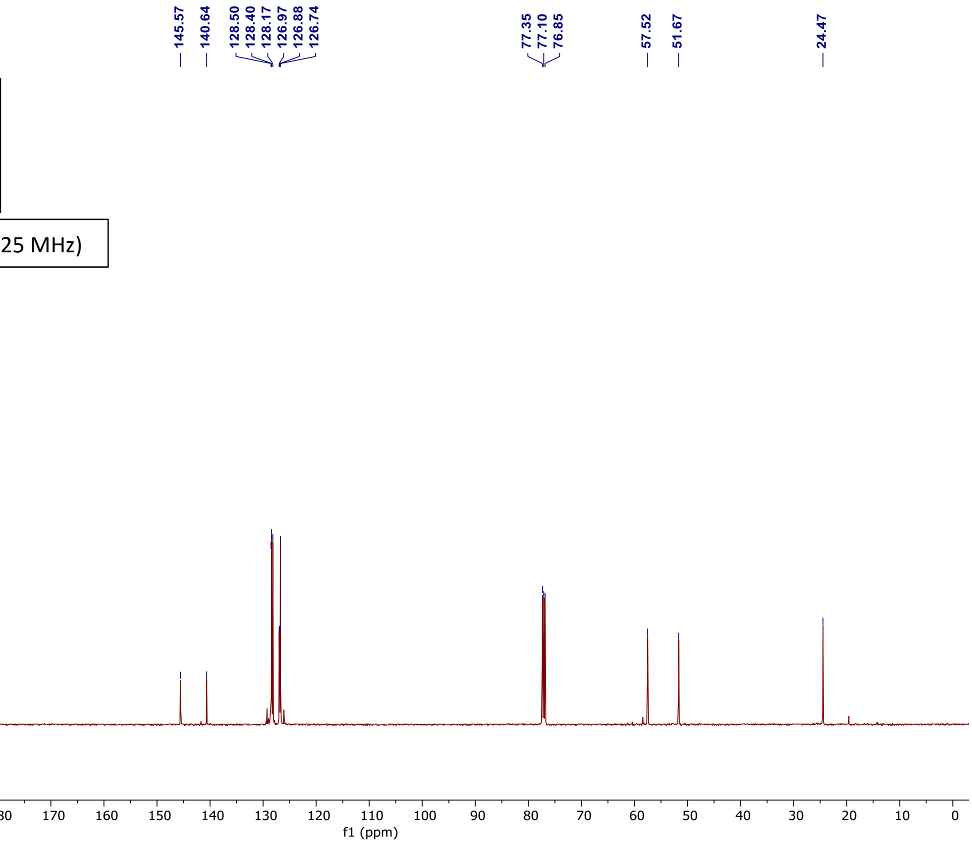


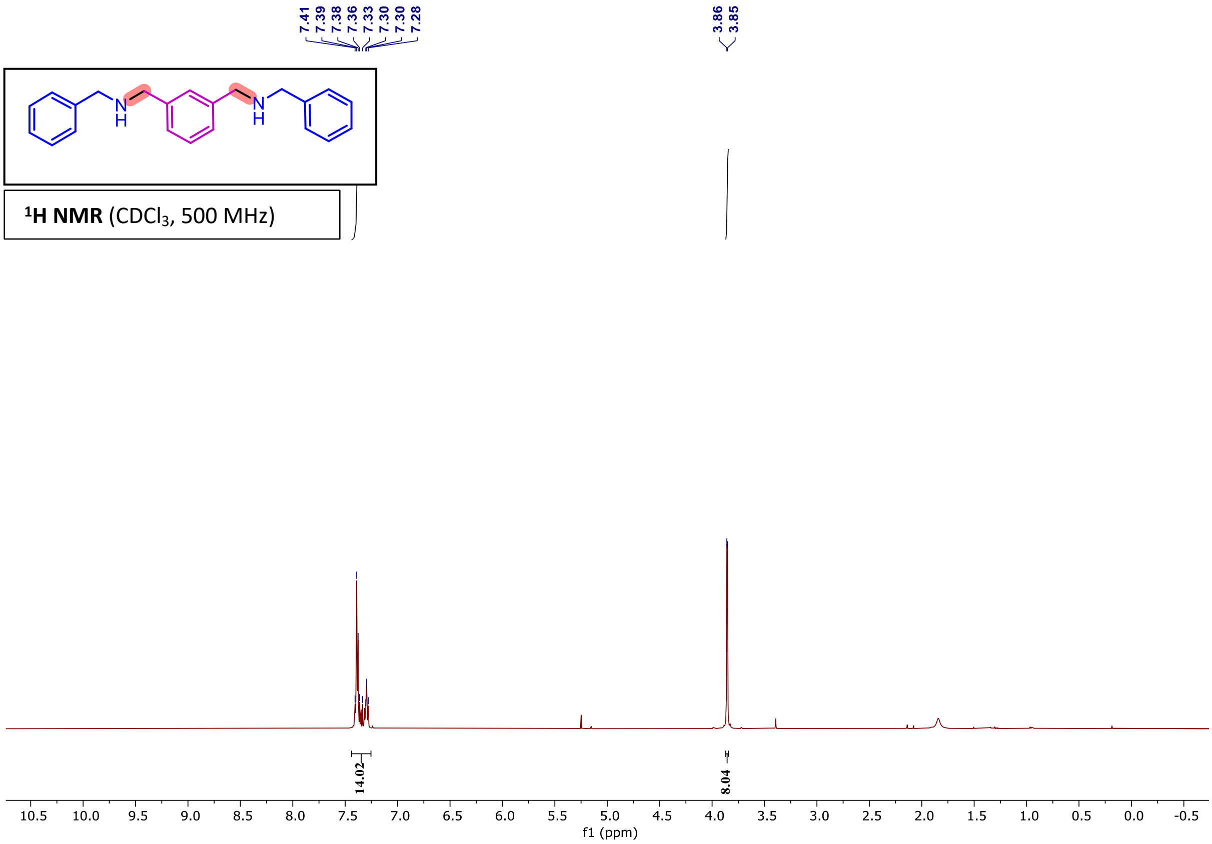
^{1}H NMR ($CDCl_3$, 500 MHz)



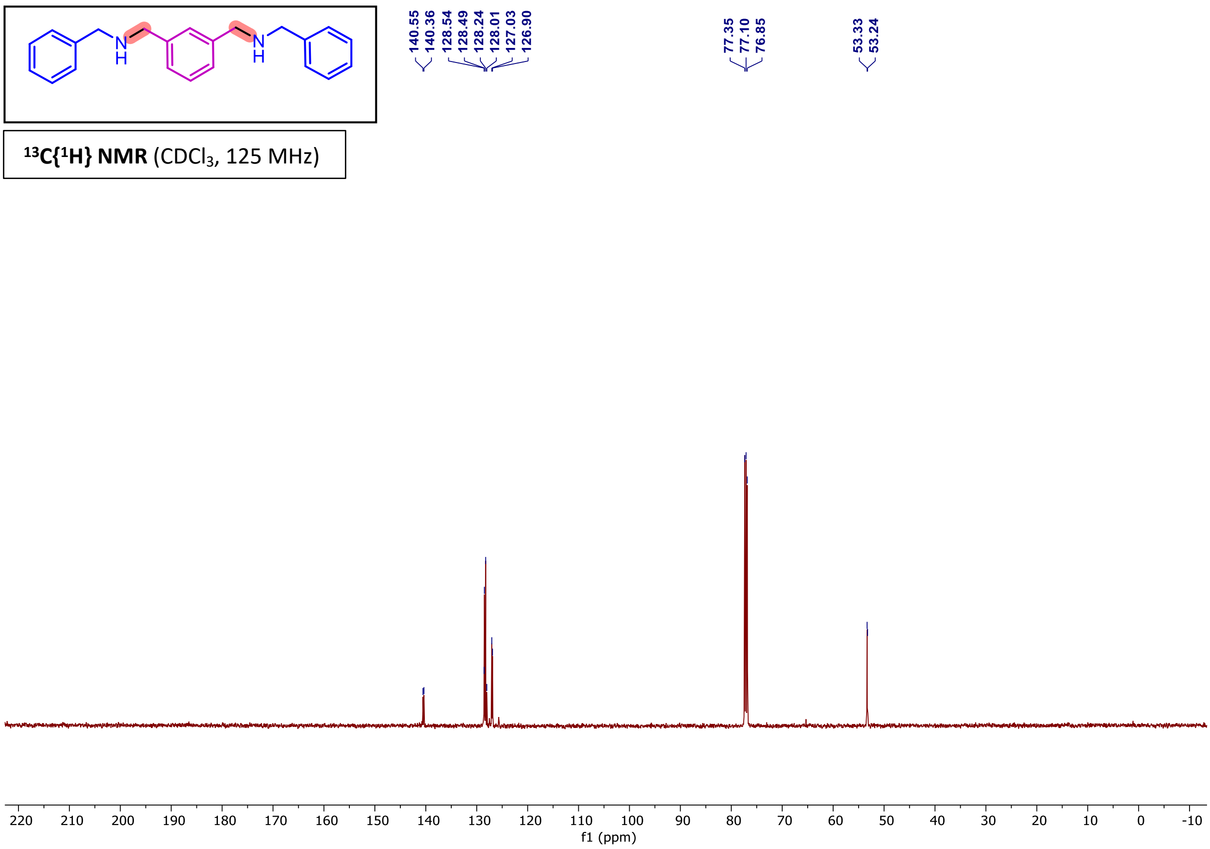


^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)





^{1}H NMR ($CDCl_3$, 500 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz)

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