Supporting Information

Ruthenium Catalyzed Synthesis of N-Methylated Amides using Methanol

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1. General Consideration

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 literature methods. Methanol was eventually distilled over sodium under argon atmosphere and deoxygenated prior to use. All the reagents were purchased from Sigma-aldrich, Alfa-acear, SD-fine chemicals, Avra Spectrochem. Synthesis of all the ruthenium complexes were reported from our group.[1] Silica gel (100-200 mesh) was used for the column chromatography with a gradient elution of hexane/ethyl acetate, based on alumina TLC plate.

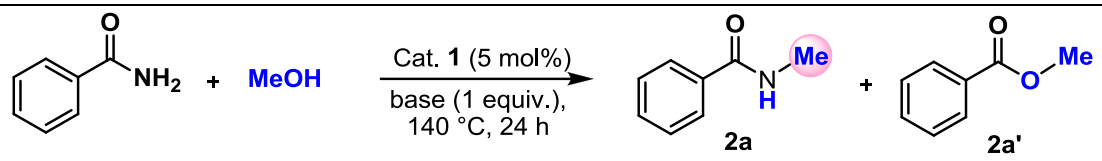
Analytical Information. ^{1}H and ^{13}C spectra were recorded on JEOL 400 MHz and 500 MHz spectrometer using $CDCl_3$ and DMSO-d_6. All ^{1}H NMR experiments were reported in parts per million (ppm) unit, and were measured relative to the signals for residual chloroform (7.24 ppm) in the deuterated 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 (77.5 ppm). 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

Reductive N-Methylation of Amide using Methanol. To an oven dried 9 mL screw cap tube a magnetic stir-bar, amide (0.5 mmol), Cs_2CO_3 (0.375 mmol), Cat. **1** (1.5 mol%) and methanol/toluene (3.0 mL, 1:5 v/v) were added under argon atmosphere. Then, the tube was sealed and placed in a preheated oil bath at 140 °C for 24 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, a small portion of the reaction mixture was diluted with EtOAc and filtered through a small plug of silica. Afterward, the sample was subjected for GC analysis to determine conversion as well as the product selectivity. Finally, the desired N-methylated amide was purified through silica gel column chromatography using hexane-ethyl acetate as eluent.

3. Optimization Details

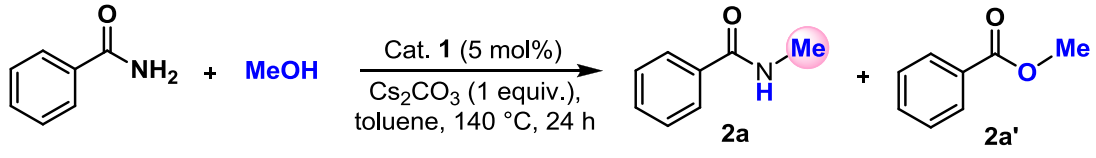
Table S1. Initial Screening of Reaction Parameters using Catalyst **1**[a]



Entry	Base (equiv.)	Conversion (%)	Yield of **2a** (%)	Yield of **2a'** (%)
1	NaOMe (1)	80	38	42
2	KO^{t}Bu (1)	77	41	36
3	Cs_2CO_3 (1)	62	42	20
4	NaOMe (0.2)	31	4	27
5	KO^{t}Bu (0.2)	23	4	19
6	Cs_2CO_3 (0.2)	34	11	23
7	K_2CO_3 (0.2)	23	5	18
8[b]	NaOMe (1)	5	1	4
9[c]	NaOMe (1)	13	3	10
10[d]	**Cs_2CO_3 (1)**	**25**	**21**	**4**

[a]Reaction conditions: benzamide (0.5 mmol), methanol (3 mL), Cat. **1** (5 mol%) and base (x equiv.) at 140 °C for 24 h; conversion and yields were determined by GC. [b]100 °C. [c]Absence of Cat. **1**. [d]Methanol/toluene (3 mL; 1:10, v/v).

Table S2. Optimization of the Amount of Methanol[a]

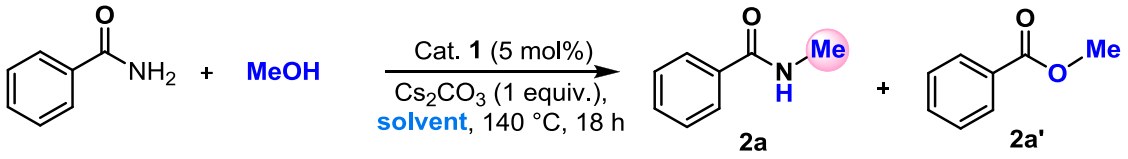


Entry	**Methanol :Toluene (v/v)**	Conversion (%)	Yield of **2a** (%)	Yield of **2a'** (%)
1	1:9	27	22	5
2	1:6	49	44	5
3	1:5	71	67	4

4	**1:4**	**99**	**91**	**8**
5	1:3	99	87	12

[a]Reaction conditions: benzamide (0.5 mmol), methanol/toluene (3 mL; 1:4, v/v), Cat. **1** (5 mol%) and Cs_2CO_3 (0.5 mmol) at 140 °C for 24 h; conversion and yields were determined by GC.

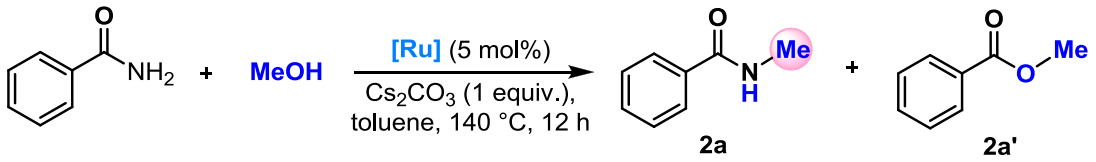
Table S3. Solvent Screening[a]



Entry	Solvent	Conversion (%)	Yield of **2a** (%)	Yield of **2a'** (%)
1	Benzene	97	87	10
2	**Toluene**	**97**	**91**	**6**
3	*m*-Xylene	77	70	7
4	Mesitylene	56	48	8
5	THF	26	25	1
6	Dioxane	14	14	0
7	DMSO	2	2	0

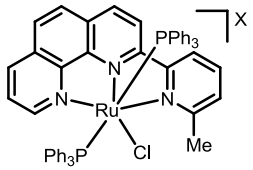
[a]Reaction conditions: benzamide (0.5 mmol), methanol/solvent (3 mL; 1:4, v/v), Cat. **1** (5 mol%) and Cs_2CO_3 (0.5 mmol) at 140 °C for 18 h; conversion and yields were determined by GC.

Table S4. Screening of Ru(II) Source[a]

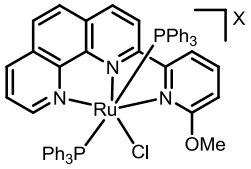


Entry	Ru (II) Catalyst	Conversion (%)	Yield of **2a** (%)	Yield of **2a'** (%)
1	**1**	**90**	**85**	**5**
2	**2**	62	54	8
3	**3**	48	41	7

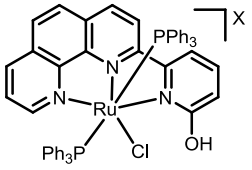
4	**4**	52	39	13
5	**5**	51	38	13
6	**6**	66	48	18
7	**7**	48	37	11
8	**8**	75	70	5
9	**9**	23	19	4
10	**10**	26	22	4
11	**11**	21	18	3
12	**12**	41	37	4
13	$RuCl_2(PPh_3)_3$	33	18	15
14	$RuHCl(CO)(PPh_3)_3$	35	21	14
15	$[RuCl_2(p\text{-cymene})]_2$	31	17	14
16	None	9	1	8



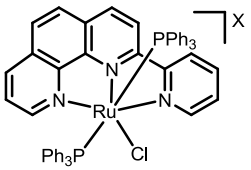
1 (X = PF_6)
2 (X = Cl)



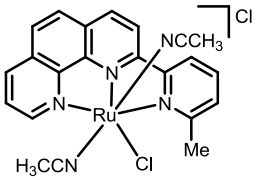
3 (X = PF_6)
4 (X = Cl)



5 (X = PF_6)
6 (X = Cl)



7 (X = PF_6)
8 (X = Cl)



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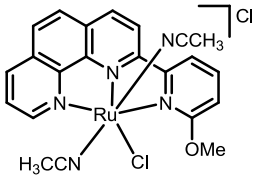

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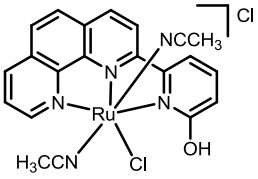

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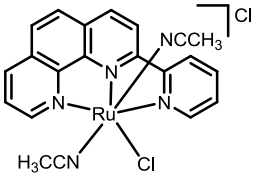
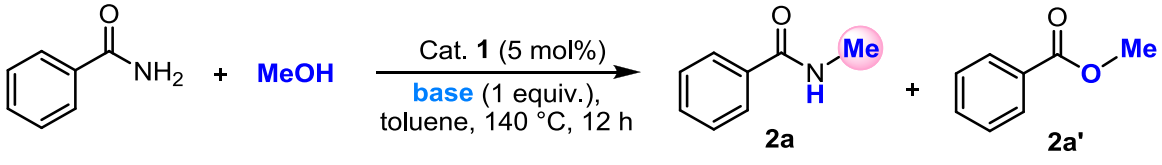


12

[a]Reaction conditions: benzamide (0.5 mmol), methanol/toluene (3 mL; 1:4, v/v), Ru(II) cat. (5 mol%) and Cs_2CO_3 (0.5 mmol) at 140 °C for 12 h; conversion and yields were determined by GC.

Table S5. Screening of Base[a]

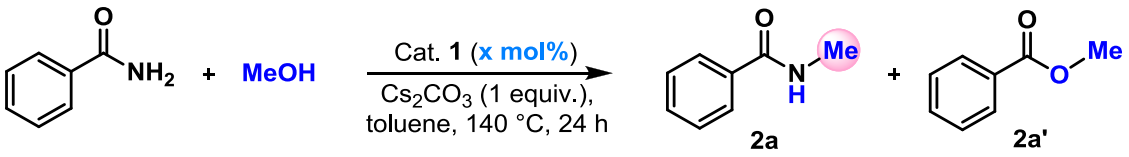


Entry	Base	Conversion	Yield of **2a**	Yield of **2a'**

		(%)	(%)	(%)
1	-			
2	Na_2CO_3	3	2	1
3	K_2CO_3	3	1	2
4	**Cs_2CO_3**	**90**	**85**	**5**
5	NaOAc	9	1	8
6	NH_4OAc	8	4	4
7	K_3PO_4	4	2	2
8	NaOH	29	10	19
9	**NaOMe**	**97**	**15**	**82**
10	NaO^iPr	19	5	14
11	NaO^tBu	32	14	18
12	LiO^tBu	45	15	30
13	KOH	6	5	1
14	KO^tBu	71	38	33

[a]Reaction conditions: benzamide (0.5 mmol), methanol/toluene (3 mL; 1:4, v/v), Cat. **1** (5 mol%) and base (0.5 mmol) at 140 °C for 12 h; conversion and yields were determined by GC.

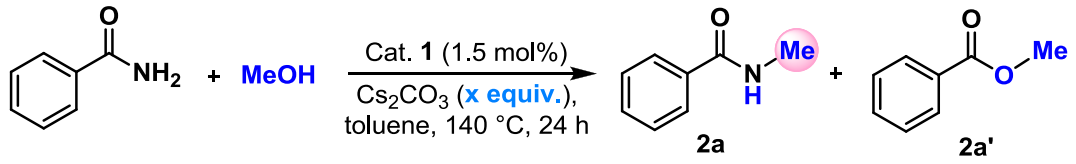
Table S6. Optimization of the Amount of Catalyst **1**[a]



Entry	Catalyst **1** **(x mol%)**	Conversion (%)	Yield of **2a** (%)	Yield of **2a'** (%)
1	0.5	65	51	14
2	1	95	82	13
3	**1.5**	**98**	**93**	**5**
4	2	100	94	6

[a]Reaction conditions: benzamide (0.5 mmol), methanol/toluene (3 mL; 1:4, v/v), Cat. **1** (x mol%) and Cs_2CO_3 (0.5 mmol) at 140 °C for 24 h; conversion and yields were determined by GC.

Table S7. Optimization of the Amount of Cs_2CO_3[a]



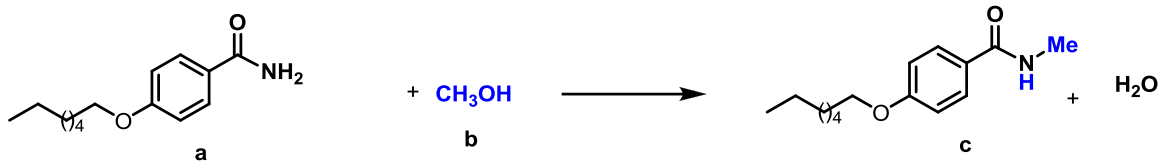
Entry	**Cs_2CO_3 (x equiv.)**	Conversion (%)	Yield of **2a** (%)	Yield of **2a'** (%)
1	0.1	21	16	5
2	0.15	72	53	19
3	0.25	81	69	12
4	0.50	94	81	13
5	**0.75**	**97**	**90**	**7**
6	1.0	98	93	5
7[b]	**0.75**	**97**	**92**	**5**

[a]Reaction conditions: benzamide (0.5 mmol), methanol/toluene (3 mL; 1:4, v/v), Cat. **1** (5 mol%) and Cs_2CO_3 (x equiv.) at 140 °C for 24 h, conversion and yields were determined by GC; [b]methanol/toluene (3 mL; 1:5, v/v).

4. Preparative Scale Reaction for the Determination of Green Chemistry Metrics

An oven dried 100 mL screw cap tube was taken inside the argon filled glove box and charged with a magnetic stir-bar, 4-(heptyloxy)benzamide (10.62 mmol), Cat. **1** (1.5 mol%), Cs_2CO_3 (7.96 mmol) followed by the addition of methanol/toluene (54.0 mL, 1:5 v/v). Then the tube was sealed and placed in a preheated oil bath at 140 °C (oil bath temperature) for 24 h. After completion of the reaction, the tube was allowed to cool at room temperature. The reaction mixture is used for the determination of green chemistry metrics[2] and the details as mentioned in the Table **S8.**

Table S8. Evaluation of Green Chemistry Metrics



Chemical Formula: $C_{11}H_{15}NO_2$
Exact Mass: 193.11

Chemical Formula: CH_4O
Exact Mass: 32.02

Total = 193.11 + 32.02 = 225.13

Chemical Formula: $C_{12}H_{17}NO_2$
Exact Mass: 207.13

Yield: 82%

Reactant **a**	4-Heptoxy benzamide	2.5 g	FW 193.11
Reactant **b**	CH_3OH	7.13 g	FW 32.02
Base	Cs_2CO_3	3.16 g	FW 325.82, 112.21
Solvent	Toluene	38.92 g	FW 106.16
Recycle solvent	-	37.5 g	-
Auxiliary	-	-	-
Product	4-(Heptyloxy)-N-methylbenzamide	2.2 g	FW 207.13

E factor = [{(2.5 g + 7.13 g + 3.16 g + 38.92 g) - (37.5 g + 2.2 g)}/2.2 g] = [(51.71 g - 39.7 g)/2.2 g] = 12.01 g/2.2 g = **5.46** kg waste/1 kg product

Atom economy = (207.13/225.13) x 100 = **92%**

Atom efficiency = 82 x (92/100) = **75.44%**

Carbon efficiency = (12/12) x 100 = **100%**

Reaction mass efficiency = [2.2g / (2.5 g + 0.41 g)] x 100 = **75.6%**

5. Time Dependent Experiment

Several experiments for the reductive N-methylation of amide were conducted following the outlined procedure with varying time. An oven dried screw cap tube was charged with benzamide (0.4 mmol), Cat. **1** (1.5 mol%), Cs_2CO_3 (0.3 mmol) followed by the addition of methanol/toluene (2.5 mL, 1:5, v/v) and mesitylene as internal standard. All the tubes were placed in a preheated oil-baths at 140 °C with stirring and the progress of the reaction was analysed by GC. All the reactions were repeated twice and the average data were plotted as conversion (%) vs time (h) (Figure **S1**).

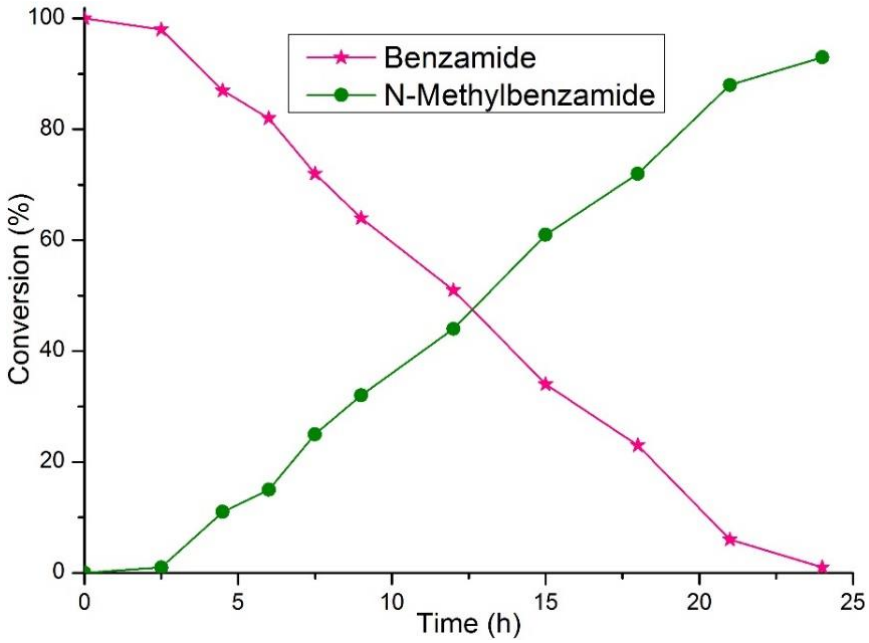


Figure S1. Time dependent product formation for benzamide.

6. Initial Rates Kinetics for the Determination of Order

Identical experiments were carried out following the general procedure varying only the amount of benzamide. 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 to determine conversion of benzamide and the yield of the N-methyl benzamide. Accordingly, the concentration of substrate and the final product were calculated at different time. All the reactions were repeated twice and the average data were plotted as

substrate cons (mM) vs time (h) in the Figure **S2**. Then, the initial rate for the different run was calculated to determine the order with respect to benzamide as mentioned bellow.

Run	Benzamide	Cs_2CO_3	Cat. **1**	Methanol/Toluene (1:5; v/v)
Run 1	0.2 mmol	0.2 mmol	3.23 mg	1.2 mL
Run 2	0.4 mmol	0.2 mmol	3.23 mg	1.2 mL

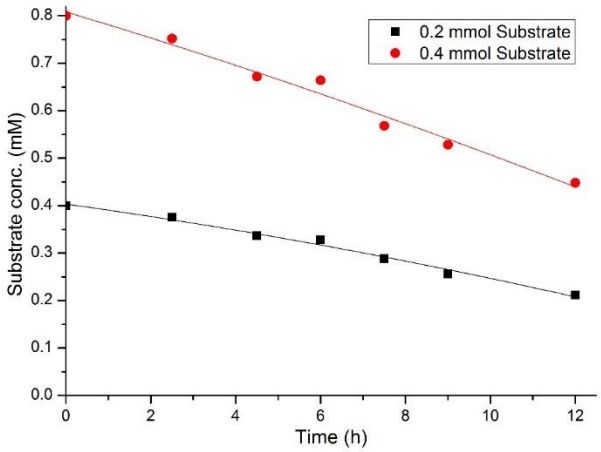


Figure S2. Determination of initial slopes for the methylation process.

Initial slope for run 1 at 4 h = 8.65 x 10^{-2} (mM)/h

Initial slope for run 2 at 4 h = 17.4 x 10^{-2} (mM)/h

Simplified rate equation for this system (r) = k[Benzamide]^a[Cs_2CO_3]^b[Cat. **1**]^c [Methanol]^d[Toluene]^e

(all term have their usual significance)

Now for run 1, r1 = 8.65 x 10^{-2} (mM)/h = k[0.2]^a[Cs_2CO_3]^b[Cat. **1**]^c [Methanol]^d[Toluene]^e …… (1)

and run 2, r2 = 17.4 x 10^{-2} (mM)/h = k[0.4]^a[Cs_2CO_3]^b[Cat. **1**]^c [Methanol]^d[Toluene]^e ……..(2)

Comparing the initial rate,

r1/r2 =8.65/17.04 = (0.2/0.4)^a

or, $0.497 = 0.5^a$; or, log 0.0.497 = a log 0.5; or, a = log 0.497/ log 0.5

or, a = -0.3036/-0.301 = 1.01 ~ 1

so, Rate = k [Benzamide]^1

7. Kinetic Isotope Effect (KIE) Studies

Parallel reactions for the reductive N-methylation were carried out using CH_3OH/toluene (1:1, v/v) and CD_3OD/toluene (1:1, v/v) under identical conditions following the outlined procedure. All the tubes were placed in a preheated oil-baths at 140 °C with stirring and the progress of the reaction was analysed by GC. All the reactions were repeated twice and the average data were plotted as yield (%) vs time (h) (Figure **S3**). All terms have their usual meaning.

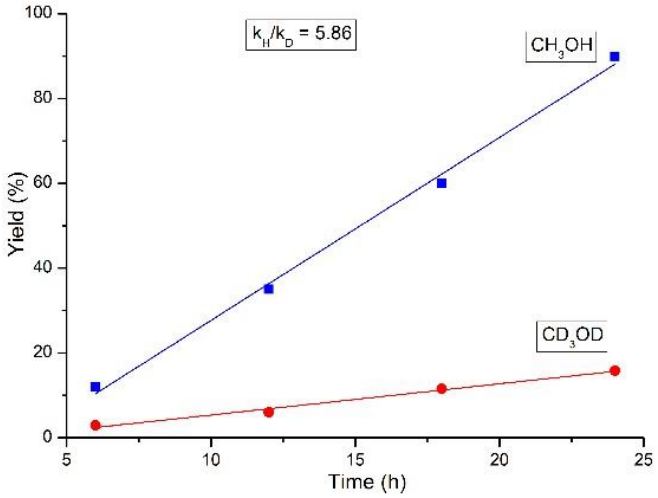


Figure S3. Kinetic isotope effect during the N-methylation of benzamide.

8. Labelling Experiments

A. Using Methanol-D_4

i) Parallel Reaction for Benzamide. Inside a argon filled glove box an oven dried 4.0 mL screw cap tube was taken and charged with benzamide or N-(hydroxymethyl)benzamide (0.2 mmol), Cat. **1** (1.5 mol%) and Cs_2CO_3 (0.15 mmol) followed by the addition of methanol-d_4/toluene (1.2 mL, 1:5 v/v). Then, the tube was sealed and placed in a preheated oil bath at 140 °C (oil bath temperature) for 72 h. The conversion of the reactions was determined by GC analysis using mesitylene as internal standard. The products were confirmed through ESI-MS analysis.

ii) Competitive Reaction for benzamide. Inside a argon filled glove box an oven dried 4.0 mL screw cap tube was taken and charged with a magnetic stir-bar, benzamide (0.2 mmol), Cat. **1** (1.5 mol%), Cs_2CO_3 (0.15 mmol) followed by the addition of methanol, methanol-d_4 and toluene (1.2 mL, 1:1:10 v/v). Then, the tube was sealed and placed in a preheated oil bath at 140 °C (oil bath temperature) for 36 h. The conversion of the reactions was determined by GC analysis using mesitylene as internal standard. The products were confirmed through ^{1}H NMR (Figure **S4**) and ESI-MS analysis (**2a**: ESI-MS calculated for C_8H_9NO; 136.0762 $(M+H)^+$, found: 136.0775. **2a1**: ESI-MS calculated for C_8H_8DNO; 137.0825 $(M+H)^+$, found: 137.0835. **2a2**: ESI-MS calculated for $C_8H_7D_2NO$; 138.0888 $(M+H)^+$, found: 138.0898. **2a3**: ESI-MS calculated for $C_8H_6D_3NO$; 139.0951 $(M+H)^+$, found: 139.0959).

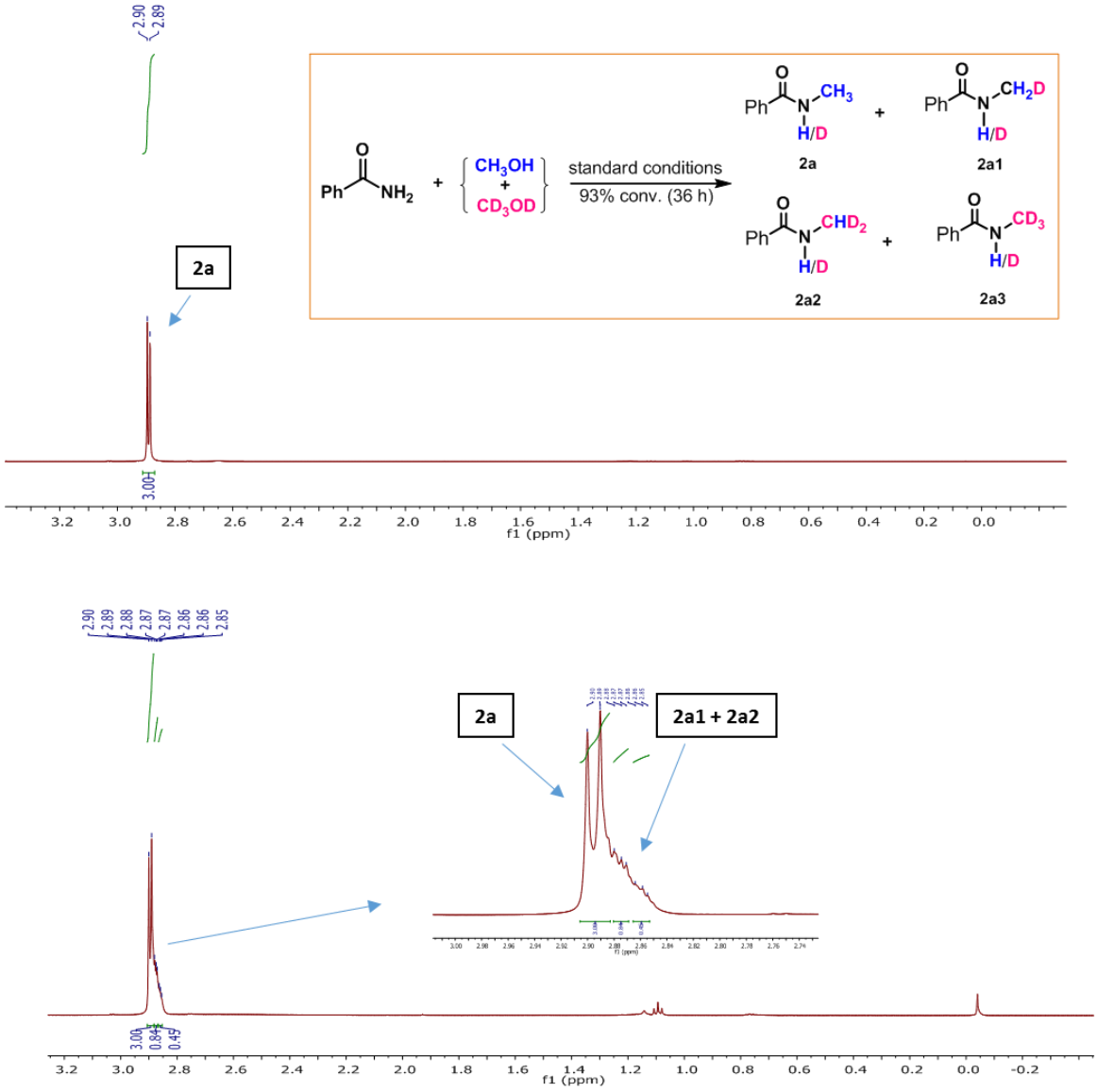


Figure S4. Partial NMR spectra of the methylated products generated from the competitive reaction.

9. Computational Studies

All the computational studies were performed using the Gaussian 09 package.[3] 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[4] for Ru and 6-31G** basis set[5] for non-metal elements (C, H, O, N and P). The transition states (TS) were further confirmed by performing intrinsic reaction coordinate (IRC) calculation using same method. In this study,

we have used methanol/toluene (1:5, v/v) for the reductive N-methylation of amide. So, the solvent effect during the calculation was not incorporated in the manuscript. In addition, calculated resultant dielectric constant of this solvent mixture was closer to THF. Therefore, indirectly solvent effect was incorporated using the conductor-like polarizable continuum model (CPCM) with THF, was shown in Figure **S5** and Figure **S6.**[6]

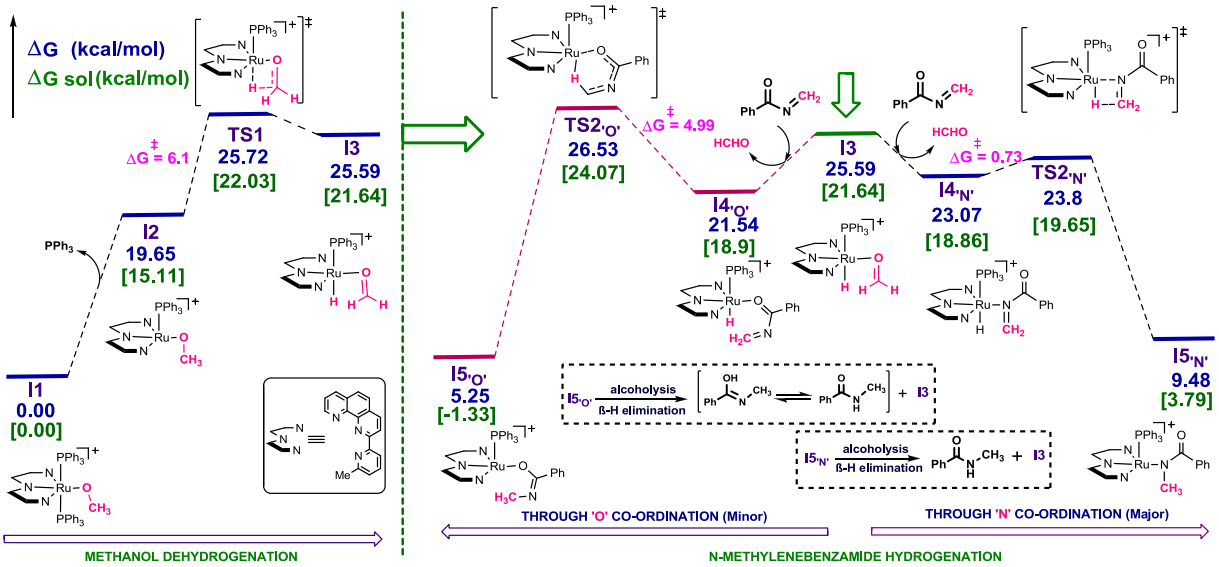


Figure S5. Computed pathway for the methanol dehydrogenation and imine insertion to ruthenium hydride by incorporating solvent correction.

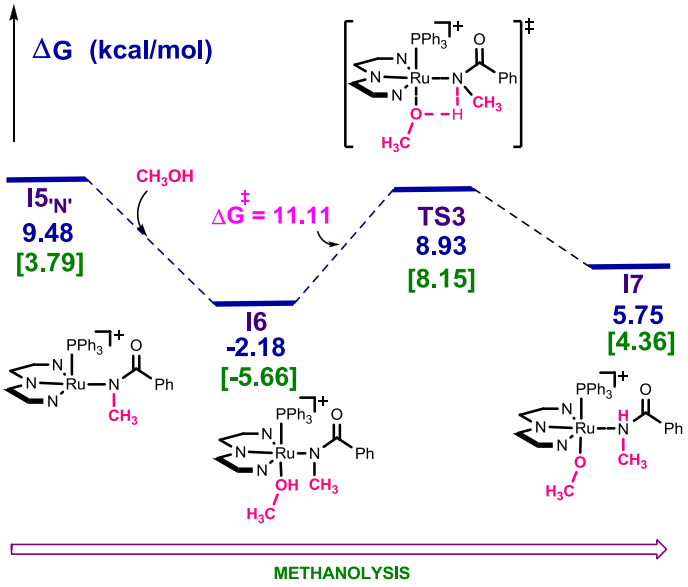


Figure S6. Computed pathway for alcoholysis by incorporating solvent correction.

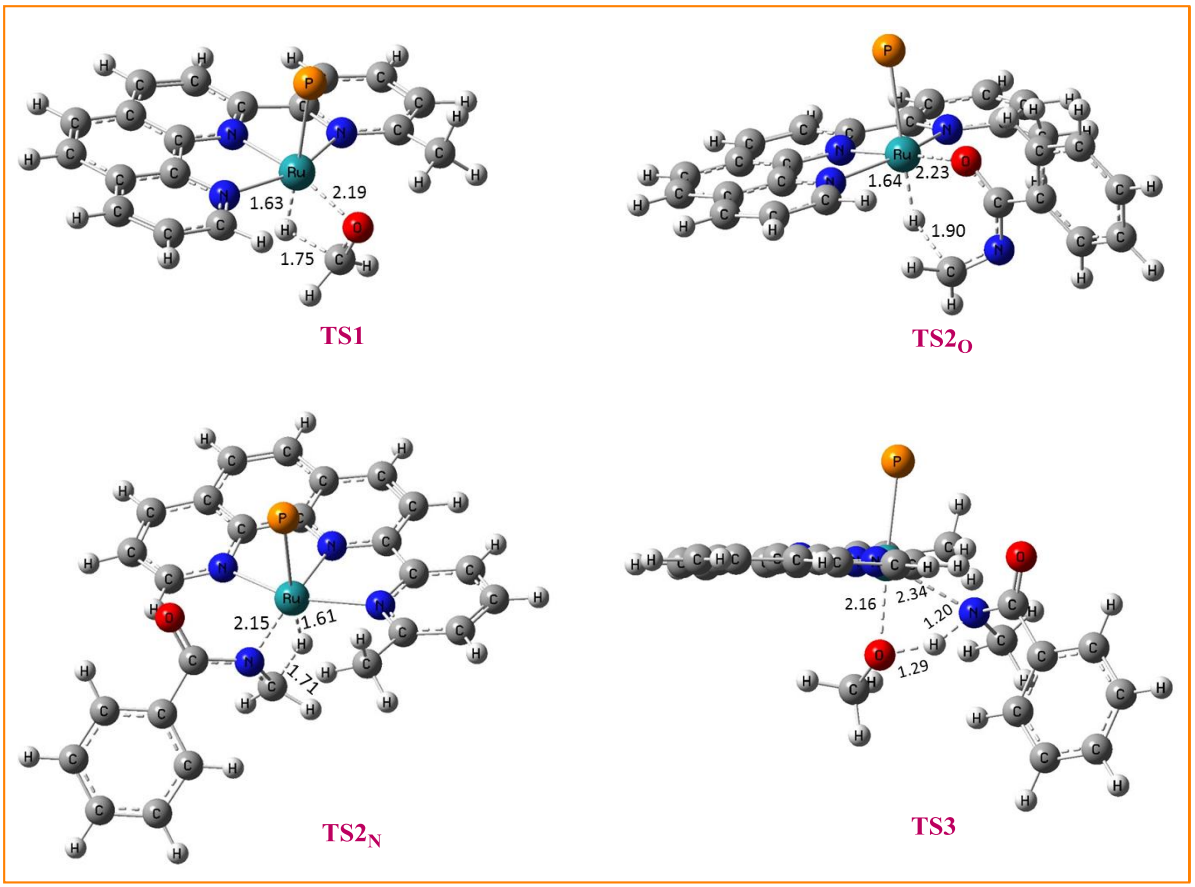
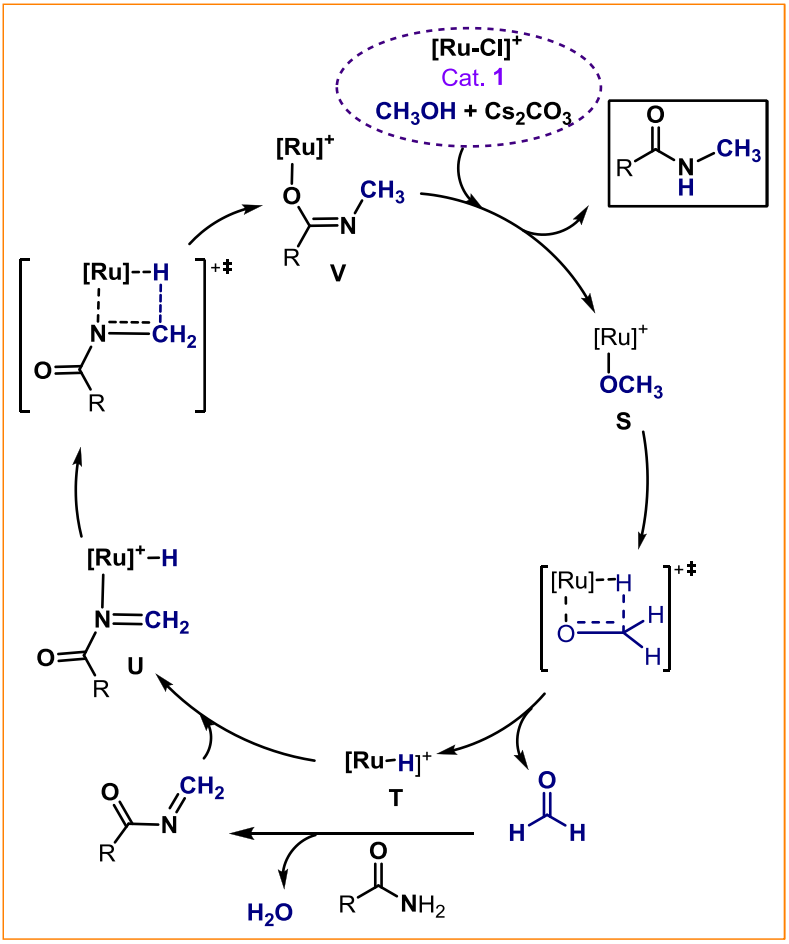


Figure S7. Optimized structure of the transition states (selected bond lengths were shown in Å and phenyl rings on the 'P' atom were removed for clarity.

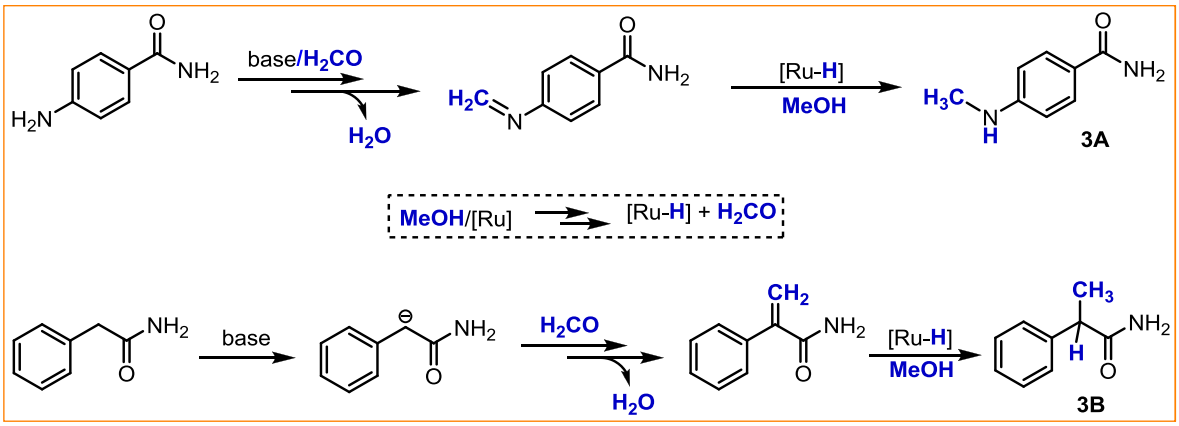
10. Plausible Mechanism

Based on the kinetic studies, control experiments and DFT calculations we proposed the mechanism for the formation of N-methylation of amides (Scheme **S1**). The species **S** was generated from the complex **1** in presence of methanol and Cs_2CO_3. Afterward, Ru-H species (**T**) and formaldehyde were produced via β-hydride elimination pathway through a four-membered **TS**. Subsequently, N-methyleneamide molecule was formed via coupling between amide and formaldehyde. Then, the resultant imine molecule was inserted to the Ru-H species preferentially via four-membered **TS**. Finally, alcoholysis of the species **V** delivered the N-methylated amide and regenerated the methoxy species **S**.



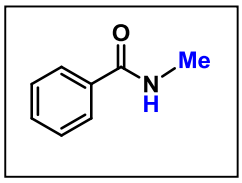
Scheme S1. Plausible mechanism for the N-methylation of amide.

In a similar way, amine N-methylation of 4-aminobenzamide and α-methylation of phenyl acetonitrile were occurred via the condensation reaction with formaldehyde and the insertion of resultant imine or olefin species to the Ru-H followed by alcoholysis (Scheme **S2**).

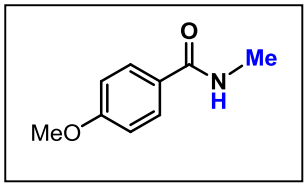


Scheme S2. Schematic pathway for the formation of **3A** and **3B**.

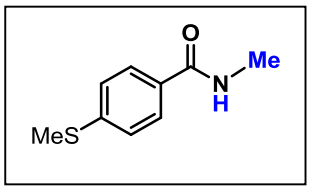
11. Spectral Data for the N-Methylated Amides



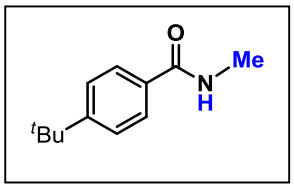
N-Methylbenzamide (2a):[7] Pale yellow solid (60.82 mg, 90% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 7.74 (d, $J_{H,H}$ = 7.5 Hz, 2H), 7.45 (t, $J_{H,H}$ = 7.25 Hz, 1H), 7.38 (t, $J_{H,H}$ = 7.75 Hz, 2H), 6.42 (brs, 1H), 2.96 (d, $J_{H,H}$ = 4.8 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 168.78, 135.07, 131.78, 128.97, 127.30, 27.28. **GC-MS** (M^+) = 135.1.



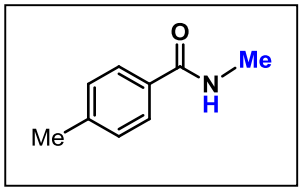
4-Methoxy-N-methylbenzamide (2b):[7] White solid (68.55 mg, 83% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.70 (d, $J_{H,H}$ = 8.8 Hz, 2H), 6.88 (d, $J_{H,H}$ = 8.9 Hz, 2H), 6.12 (brs, 1H), 3.82 (s, 3H), 2.97 (d, $J_{H,H}$ = 4.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 168.25, 162.51, 129.07, 127.37, 114.18, 55.86, 27.27. **GC-MS** (M^+) = 165.1.



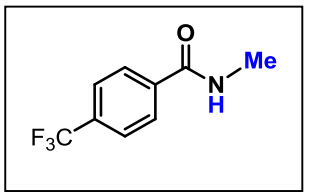
N-Methyl-4-(methylthio)benzamide (2c):[8] White solid (77.0 mg, 85% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 7.65 (d, $J_{H,H}$ = 8.5 Hz, 2H), 7.24-7.22 (m, 2H, overlapped with $CDCl_3$), 6.08 (brs, 1H), 2.98 (d, $J_{H,H}$ = 4.8 Hz, 3H), 2.48 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 168.14, 143.73, 131.26, 127.71, 125.97, 27.31, 15.56. **GC-MS** (M^+) = 181.1.



4-Tert-butyl-N-methylbenzamide (2d):[7] Pale yellow solid (74.6 mg, 78% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 7.67 (d, $J_{H,H}$ = 8.2 Hz, 2H), 7.41 (d, $J_{H,H}$ = 8.2 Hz, 2H), 6.18 (brs, 1H), 2.98 (d, $J_{H,H}$ = 4.8 Hz, 3H), 1.30 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 168.68, 155.28, 132.24, 127.13, 125.95, 35.37, 31.64, 27.26. **GC-MS** (M^+) = 191.1.

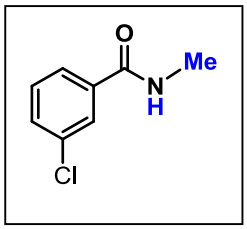


N,4-Dimethylbenzamide (2e):[7] White solid (52.96 mg, 71% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.64 (d, $J_{H,H}$ = 8.2 Hz, 2H), 7.15 (d, $J_{H,H}$ = 8 Hz, 2H), 6.55 (brs, 1H,), 2.93 (d, $J_{H,H}$ = 4.8 Hz, 3H), 2.33 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 168.69, 142.01, 132.14, 129.53, 127.31, 27.17, 21.80. **GC-MS** (M^+) = 149.1.

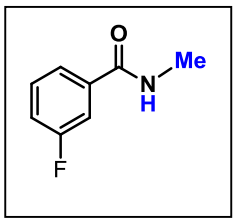


N-Methyl-4-(trifluoromethyl)benzamide (2f):[7] White solid (85.33 mg, 84% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.83 (d, $J_{H,H}$ = 8.2 Hz, 2H), 7.54 (d, $J_{H,H}$ = 8.2 Hz, 2H), 7.40 (brs, 1H), 2.86

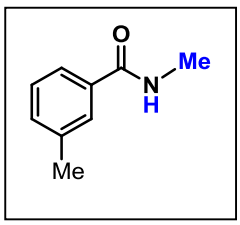
(d, $J_{H,H}$ = 4.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 167.23, 138.32, 133.09, 132.76, 127.92, 125.58, 27.08. **GC-MS** (M^+) = 203.1.



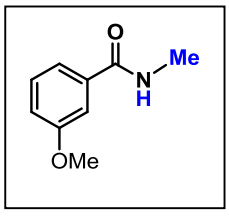
3-Chloro-N-methylbenzamide (2g):[9] White solid (78.86 mg, 93% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 7.72 (t, $J_{H,H}$ = 1.8 Hz, 1H), 7.60 (dt, $J_{H,H}$ = 7.75, 1.0 Hz, 1H), 7.36 (d, $J_{H,H}$ = 7.9 Hz, 1H), 7.25 (t, $J_{H,H}$ = 7.8 Hz, 1H), 7.1 (brs, 1H), 2.91 (d, $J_{H,H}$ = 4.8 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 167.62, 136.67, 134.93, 131.69, 130.15, 127.72, 125.47, 27.31. **GC-MS** (M^+) = 169.0.



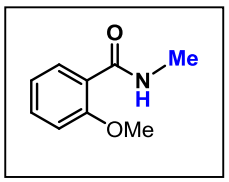
3-Fluoro-N-methylbenzamide (2h):[10] White solid (63.56 mg, 83% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.50-7.45 (m, 2H,), 7.37-7.32 (m, 1H), 7.17-7.12 (m, 1H,), 6.52 (brs, 1H), 2.96 (d, $J_{H,H}$ = 4.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 167.57, 164.40, 161.93, 137.26 (d, J = 7 Hz), 130.64 (d, J = 8 Hz), 122.81 (d, J = 3 Hz), 118.80 (d, J = 21 Hz), 114.75 (d, J = 23 Hz), 27.37. **GC-MS** (M^+) = 153.1.



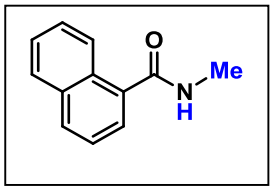
N,3-Dimethylbenzamide (2i):[11] Pale yellow oil (63.40 mg, 85% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.56 (s, 1H), 7.52-7.49 (m, 1H), 7.25 (d, $J_{H,H}$ = 4.9 Hz, 2H), 6.41 (brs, 1H), 2.96 (d, $J_{H,H}$ = 4.9 Hz, 3H), 2.34 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 168.98, 138.77, 135.0, 132.48, 128.81, 128.09, 124.23, 27.25, 21.77. **GC-MS** (M^+) = 149.1.



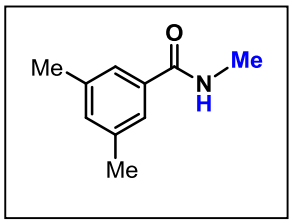
3-Methoxy-N-methylbenzamide (2j):[12] Colourless liquid (64.42 mg, 78% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.33-7.27 (m, 2H), 7.25-7.23 (m, 1H, overlapped with $CDCl_3$), 7.01-6.98 (m, 1H), 6.24 (brs, 1H), 3.81 (s, 3H), 2.97 (d, $J_{H,H}$ = 4.8 Hz, 3H) . **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 168.59, 160.25, 136.56, 130.0, 119.02, 118.04, 112.67, 55.87, 27.34. **GC-MS** (M^+) = 165.1.



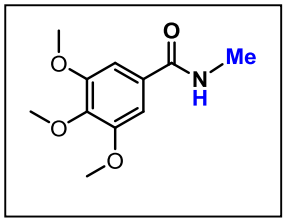
2-Methoxy-N-methylbenzamide (2k):[13] Colourless oil (42.95 mg, 52% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 8.18 (dd, $J_{H,H}$ = 7.8, 1.8 1H), 7.81 (brs, 1H), 7.41-7.38 (m, 1H), 7.05-7.02 (m, 1H), 6.93 (d, $J_{H,H}$ = 8.2 Hz, 1H), 3.92 (s, 3H), 2.97 (d, $J_{H,H}$ = 4.8 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$**)** δ = 166.42, 157.83, 133.05, 132.65, 121.91, 121.67, 111.64, 56.31, 26.98. **GC-MS** (M^+) = 165.1.



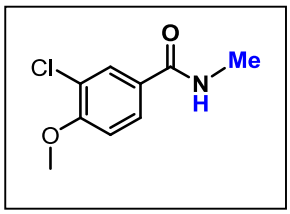
N-Methyl-1-naphthamide (2l):[10] Pale yellow solid (59.27 mg, 64% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 8.27-8.25 (m, 1H), 7.88-7.82 (m, 2H), 7.55-7.49 (m, 3H), 7.42-7.38 (m, 1H), 6.04 (brs, 1H), 3.04 (d, $J_{H,H}$ = 4.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 170.74, 135.03, 134.11, 131.61, 130.98, 130.56 128.74, 127.52, 126.87, 125.88, 125.32, 125.17, 27.31. **GC-MS** (M^+) = 185.1.



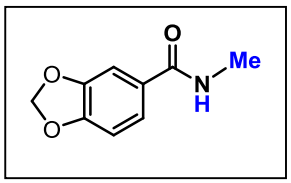
N,3,5-Trimethylbenzamide (2m):[14] White solid (67.73 mg, 83% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.33 (s, 2H), 7.08 (s, 1H), 6.26 (brs, 1H), 2.96 (d, $J_{H,H}$ = 4.8 Hz, 3H), 2.30 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 169.14, 138.63, 135.06, 133.35, 125.08, 27.24, 21.67 .**GC-MS** (M^+) = 163.1.



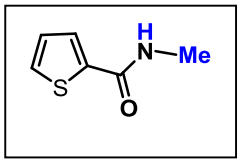
3,4,5-Trimethoxy-N-methylbenzamide (2n):[7] White solid (68.70 mg, 61% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 6.96 (s, 2H), 6.31 (brs, 1H), 3.85 (s, 6H), 3.84 (s, 3H), 2.96 (d, $J_{H,H}$ = 4.8 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 168.46, 153.59, 141.09, 130.57, 104.63, 61.35, 56.68, 27.38. **GC-MS** (M^+) = 225.1.



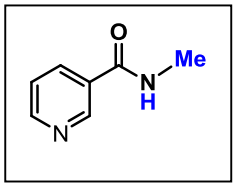
3-Chloro-4-methoxy-N-methylbenzamide (2o): Yellowish liquid (83.84 mg, 84% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.77 (d, $J_{H,H}$ = 2.0 Hz, 1H), 7.65 (dd, $J_{H,H}$ = 8.6, 2.08 Hz, 1H), 6.92 (d, $J_{H,H}$ = 8.6 Hz, 1H), 6.10 (brs, 1H), 3.92 (s, 3H), 2.97 (d, $J_{H,H}$ = 4.9 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 167.09, 157.86, 129.46, 128.20, 127.41, 123.07, 111.95, 56.78, 27.36. **ESI-MS:** Calculated for $C_9H_{10}ClNO_2$; 200.0478 $(M+H)^+$, found: 200.0473.



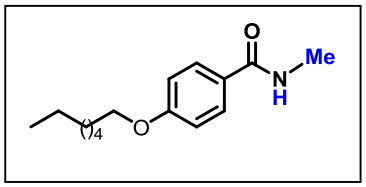
N-Methylbenzo[d][1,3]dioxole-5-carboxamide (2p):[15] Yellowish solid (55.54 mg, 62% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.27-7.24 (m, 2H), 6.77 (d, $J_{H,H}$ = 7.9 Hz, 1H), 6.20 (brs, 1H), 5.98 (s, 2H), 2.94 (d, $J_{H,H}$ = 4.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ= 168.02, 150.64, 148.37, 129.29, 121.85, 108.42, 108.03, 102.09, 27.34. **GC-MS** (M^+) = 179.1.



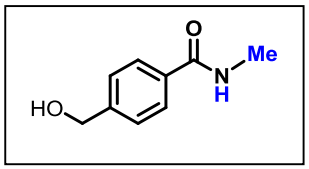
N-Methylthiophene-2-carboxamide (2q):[7] Yellowish solid (45.88 mg, 65% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 7.54 (d, $J_{H,H}$ =3.5 Hz, 1H), 7.40 (d, $J_{H,H}$ =4.8 Hz, 1H), 7.01 (t, $J_{H,H}$ =4.6 Hz, 1H), 6.54 (brs, 1H), 2.94 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 163.20, 139.47, 130.08, 128.50, 128.07, 27.15. **GC-MS** (M^+) = 141.1.



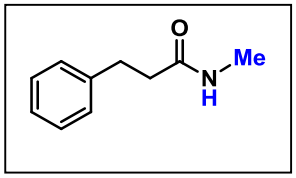
N-Methylnicotinamide (2r):[8] Brown solid (59.22 mg, 87% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 8.88 (s, 1H), 8.49 (d, $J_{H,H}$ = 3.9 Hz, 1H), 7.99 (d, $J_{H,H}$ = 8 Hz, 1H), 7.73 (brs, 1H), 7.20-7.17 (m, 1H), 2.79 (d, $J_{H,H}$ = 4.7 Hz, 3H) . **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 166.49, 151.84, 148.59, 135.30, 130.57, 123.42, 26.84. **GC-MS** (M^+) = 136.1.



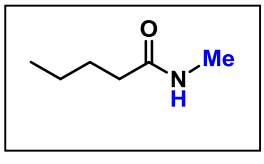
4-(Heptyloxy)-N-methylbenzamide (2s): Pale yellow oil (108.47 mg, 87% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.68 (d, $J_{H,H}$ = 8.7 Hz, 2H), 6.87 (d, $J_{H,H}$ = 8.8 Hz, 2H), 6.06 (brs, 1H), 3.96 (t, $J_{H,H}$ = 6.6 Hz, 2H), 2.97 (d, $J_{H,H}$ = 4.9 Hz, 3H), 1.78-1.73 (m, 2H), 1.64 (brs, 1H), 1.43-1.29 (m, 9H), 0.88-0.85 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 168.28, 162.17, 129.02, 127.14, 114.70, 68.65, 32.24, 29.57 (d, J = 12), 27.26, 26.44, 23.08, 14.56. **ESI-MS:** Calculated for $C_{15}H_{23}NO_2$; 250.1807 $(M+H)^+$, found: 250.1809.



4-(Hydroxymethyl)-N-methylbenzamide (2t):[16] Yellowish solid (67.72 mg, 82% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.68 (d, $J_{H,H}$ = 8.1 Hz, 2H), 7.35 (d, $J_{H,H}$ = 8.0 Hz, 2H), 6.26 (brs, 1H), 4.70 (s, 2H), 2.98 (d, $J_{H,H}$ = 4.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 168.61, 144.95, 134.08, 127.51, 127.23, 65.05, 27.33. **GC-MS** (M^+) = 165.1.

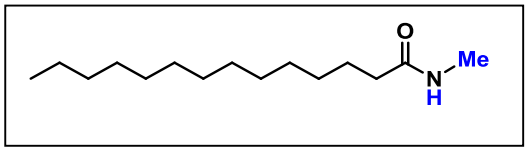


N-Methyl-3-phenylpropanamide (2u):[17] Colourless oil (60.39 mg, 74% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 7.25-7.22 (m, 2H), 7.17 -7.14 (m, 3H), 6.01 (brs, 1H), 2.91 (t, $J_{H,H}$ = 8.1 Hz, 2H), 2.70 (d, $J_{H,H}$ = 4.8 Hz, 3H), 2.43 (t, $J_{H,H}$ = 8.1 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 173.38, 141.30, 128.85, 128.63, 126.55, 38.62, 32.13, 26.60. **GC-MS** (M^+) = 163.1.

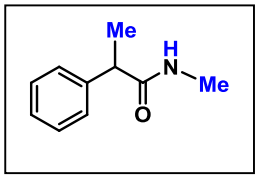


N-Methylpentanamide (2v):[18] Colourless oil (48.95 mg, 85% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 5.76 (s, 1H), 2.75 (d, $J_{H,H}$ = 4.8 Hz, 3H), 2.13 (t, $J_{H,H}$ = 7.4 Hz, 2H), 1.60-1.52 (m, 2H), 1.34-1.24 (m, 2H),

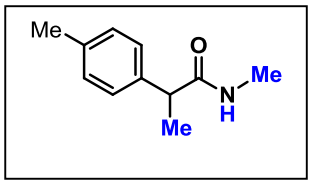
0.86 (t, $J_{H,H}$ = 7.4 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 174.41, 36.83, 28.31, 26.66, 22.85, 14.22. **GC-MS** (M^+) = 115.1.



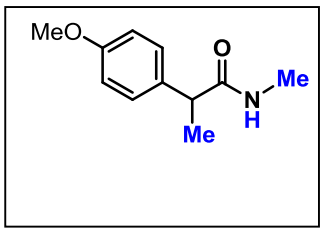
N-Methyltetradecanamide (2w):[19] Colourless oil (85.70 mg, 71% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 5.55 (brs, 1H), 2.77 (d, $J_{H,H}$ = 4.8 Hz, 3H), 2.13 (t, $J_{H,H}$ = 7.8 Hz, 2H), 1.61-1.56 (m, 2H), 1.22 (brs, 20H), 0.84 (t, $J_{H,H}$ = 6.8 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 174.34, 37.22, 32.39, 30.12 (t, J = 3.1), 29.96, 29.82, 26.73, 26.27, 23.16, 14.59. **GC-MS** (M^+) = 241.2.



N-Methyl-2-phenylpropanamide (2x):[20] White solid (66.92 mg, 82% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.28-7.22 (m, 4H), 7.20-7.16 (m, 1H), 5.88 (brs, 1H), 3.50 (q, $J_{H,H}$ = 7.2 Hz, 1H), 2.64 (d, $J_{H,H}$ = 4.8 Hz, 3H), 1.44 (d, $J_{H,H}$ = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 175.33, 141.84, 129.12, 127.96, 127.48, 47.20, 26.77, 18.87. **ESI-MS:** Calculated for $C_{10}H_{13}NO$; 164.1075 $(M+H)^+$, found: 164.1071.



N-Methyl-2-p-tolylpropanamide (2y):[21] Light yellow oil (63.80 mg, 72% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.17-7.10 (m, 4H), 5.80 (brs, 1H), 3.50 (q, $J_{H,H}$ = 7.2 Hz, 1H), 2.68 (d, $J_{H,H}$ = 4.8 Hz, 3H), 2.29 (s, 3H), 1.46 (d, $J_{H,H}$ = 7.2 Hz, 3H) . **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 175.52, 138.80, 137.13, 129.83, 127.86, 46.82, 26.77, 21.36, 18.87. **ESI-MS:** Calculated for $C_{11}H_{15}NO$; 178.1232 $(M+H)^+$, found: 178.1236.

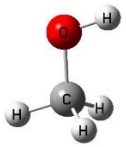


2-(4-Methoxyphenyl)-N-methylpropanamide (2z): Light yellow oil (67.63 mg, 70% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 7.17 (d, $J_{H,H}$ = 8.6, 2H), 6.83 (d, $J_{H,H}$ = 8.7, 2H), 5.54 (brs, 1H), 3.75 (s, 3H), 3.47 (q, $J_{H,H}$ = 7.2, 1H), 2.68 (d, $J_{H,H}$ = 4.8, 3H), 1.45 (d, $J_{H,H}$ = 7.2, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 175.71, 159.17, 133.83, 129.12, 114.67, 55.70, 46.57, 26.88, 19.0. **ESI-MS:** Calculated for $C_{11}H_{15}NO_2$; 194.1181$(M+H)^+$, found: 194.1189.

12. Cartesian Coordinates and Statistical Thermodynamic Analysis

(Energy in Hartree Unit)

Methanol



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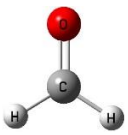
SCF done for solvent	-115.66670165
Zero-point correction	0.052277
Thermal correction to Gibbs free energy	0.029621

C	0.65811300	-0.01987600	0.00000400
H	1.08140600	0.98663500	-0.00109700
H	1.02898000	-0.54316800	0.89180800
H	1.02880000	-0.54500600	-0.89078600
O	-0.74417100	0.12221900	0.00000600
H	-1.13449400	-0.75695200	0.00000700

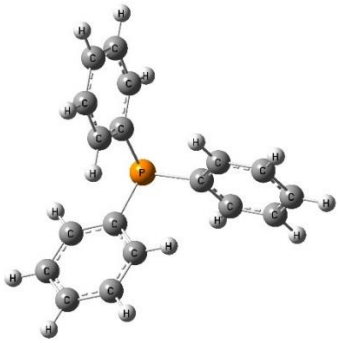
Formaldehyde



SCF done	-114.44715561
SCF done for solvent	-114.45118624
Zero-point correction	0.027267
Thermal correction to Gibbs free energy	0.005613

C	0.52714800	-0.00000100	-0.00003800
O	-0.67404600	-0.00002200	0.00000900
H	1.11490500	-0.93812200	0.00007700
H	1.11456900	0.93830200	0.00007700

Triphenylphosphine



SCF done	-1035.96764575
SCF done for solvent	-1035.97370210
Zero-point correction	0.276350
Thermal correction to Gibbs free energy	0.232323

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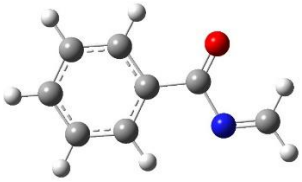
C	2.34473300	-3.47439400	0.71436300
C	1.75101500	-1.13310100	0.69230500
C	2.41919200	3.18127600	-0.41931500
C	1.56705900	-3.67997600	-0.42277100
C	1.82932000	2.06232900	-0.99799600
C	0.96771800	-1.32923700	-0.44945100
C	1.84504000	3.76608200	0.70728900
C	0.89172100	-2.61207800	-1.00471200
C	0.66854700	1.50150800	-0.45066000
C	0.68413300	3.22386100	1.25165400
C	0.09942100	2.09638600	0.67907900
C	-1.85940400	-0.93862200	0.70321300
C	-1.63808300	-0.17537300	-0.44711400
C	-3.12826700	-0.99716200	1.27565900
C	-2.71127800	0.52437400	-1.01120400
C	-4.18642400	-0.28906800	0.71230300
C	-3.97544900	0.47574700	-0.43244600
H	3.04444200	-2.03443800	2.15216600
H	2.88008900	-4.30383900	1.16563100
H	1.82473900	-0.14316900	1.13323300
H	3.32108600	3.60236400	-0.85229900
H	2.27208800	1.61561200	-1.88501700
H	1.49359100	-4.66996900	-0.86181900
H	2.29825100	4.64464400	1.15534700
H	0.29684800	-2.77269300	-1.90076300
H	-1.03786300	-1.48939700	1.15263900
H	0.23153800	3.67812900	2.12760000
H	-0.80288600	1.67720600	1.11443100
H	-3.28960600	-1.59652900	2.16642700
H	-2.55136000	1.11072700	-1.91287400
H	-5.17359400	-0.33698900	1.16105300
H	-4.79677000	1.02680300	-0.87982200
P	-0.00322900	-0.00150200	-1.28279700

N-Methylenebenzamide



SCF done	-438.83519701
SCF done for solvent	-438.84053886
Zero-point correction	0.133164
Thermal correction to Gibbs free energy	0.100451

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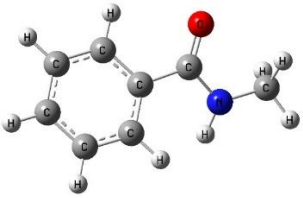
C	0.66660900	-1.18274800	-0.00016100
C	2.04488800	-1.37533500	-0.00004100
C	2.90308100	-0.27873400	0.00014300
C	2.38769300	1.01810900	0.00020500
C	1.01425300	1.21564400	0.00008100
H	-0.01827300	-2.02228000	-0.00030800
H	2.44966300	-2.38205700	-0.00009000
H	3.97763100	-0.43335800	0.00023600
H	3.05923600	1.87025000	0.00035000
H	0.58487200	2.21206900	0.00012300
O	-1.77864300	1.49295200	-0.00030700
C	-1.31278100	0.37587200	-0.00022400
C	-3.37386000	-0.61220800	0.00037600
H	-3.79828000	0.39679600	0.00146900
H	-4.05004000	-1.46648700	0.00081400
N	-2.12234300	-0.82510300	-0.00025700

N-Methylbenzamide



SCF done	-440.07502409
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Zero-point correction	0.157895
Thermal correction to Gibbs free energy	0.123398

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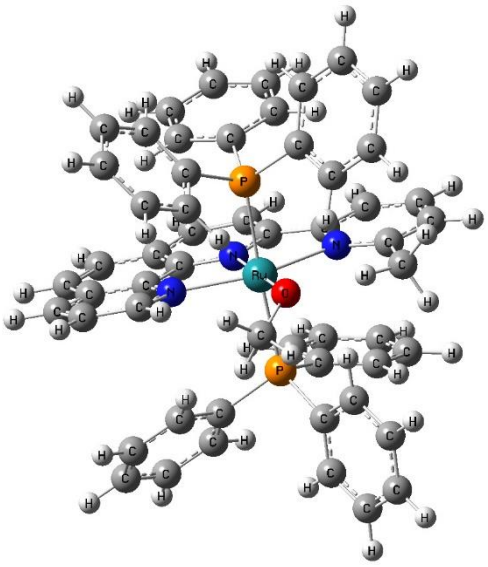
C	0.24501600	0.10211700	-0.05070300
C	1.08488400	1.19932100	0.14249700
C	0.79537100	-1.17251500	-0.20176100
C	2.46125400	1.02130400	0.21229700
H	0.63243500	2.18136900	0.23122200
C	2.17445600	-1.34884000	-0.13863200
H	0.15480600	-2.02546000	-0.40780500
C	3.00734700	-0.25378700	0.07521000
H	3.11106200	1.87591100	0.37089000
H	2.59920600	-2.33926900	-0.26615900
H	4.08254500	-0.39313000	0.12630100
C	-3.48149900	-0.49588200	0.19694400
H	-3.77171000	0.12951500	-0.64739400
O	-1.67290100	1.47584600	-0.38607000
H	-3.98053000	-1.46294700	0.12116000
H	-1.65229000	-1.48567500	0.63028400

I1



SCF done	-3138.44333303
SCF done for solvent	-3138.49158362
Zero-point correction	0.874815
Thermal correction to Gibbs free energy	0.788278

C	0.00517000	4.80693500	-0.75839200
C	-0.21365700	4.13337100	-1.93748200
C	0.31617300	4.67795500	1.72885700
C	0.14576400	4.07001400	0.43607800
C	0.37751300	3.93232400	2.86418700
C	-0.26375400	2.72690400	-1.93373900
C	0.08186500	2.66903800	0.34146100

C	0.28175700	2.50178600	2.80428600
C	0.16586800	1.89275400	1.54718300
C	0.24800200	1.64451400	3.92867300
C	0.10444000	0.28584700	3.76250500
C	0.02692600	-0.25314900	2.45829700
C	-0.04412800	-1.69372300	2.11735300
C	-0.08662300	-3.29921600	0.43112000
C	-0.05576100	-2.66530300	3.10747400
C	-0.11332100	-4.31979400	1.39351200
C	-0.10281100	-4.00593400	2.73807900
H	0.05473900	5.89145000	-0.73184300
H	-0.34705100	4.66142800	-2.87420100
H	0.37788400	5.76060700	1.77979900
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H	-0.41715500	2.17262300	-2.85235100
H	0.31907100	2.06929200	4.92547900
H	0.06344300	-0.36346300	4.62802100
H	-0.02668600	-2.38483200	4.15281700
H	-0.13577100	-5.35059300	1.05677500
H	-0.12075700	-4.78535700	3.49257200
N	-0.10604500	2.00361000	-0.83631900
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Ru	-0.08620500	-0.15579900	-0.49008200
O	-0.29299400	-0.87151200	-2.49895700
C	0.28353300	-0.20562700	-3.56449900
H	1.19086000	0.36999100	-3.29112200
H	0.60065000	-0.90483700	-4.35650700
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P	2.43057300	-0.24647600	-0.51623200
P	-2.48762100	-0.17424100	-0.34650500
C	3.34572500	-1.20430200	-1.78059300
C	2.65238900	-2.06264800	-2.63571500
C	4.74343600	-1.13960900	-1.83982800
C	3.35567500	-2.85828300	-3.54020200
H	1.56772400	-2.08130500	-2.60195600
C	5.43768900	-1.93253900	-2.74492200
H	5.28708600	-0.46870300	-1.17972900
C	4.74378500	-2.79535700	-3.59392200
H	2.81278100	-3.51981800	-4.20795400
H	6.52041200	-1.87838100	-2.79020500
H	5.28980300	-3.41243100	-4.30023600
C	3.30636300	1.37311400	-0.53195600
C	4.34724700	1.73121800	0.33155400
C	2.92359200	2.27567800	-1.53193900
C	4.95280800	2.98227000	0.22446300
H	4.70136000	1.03365800	1.08303600
C	3.52588200	3.52385800	-1.63708300
H	2.16013600	1.98580200	-2.24646100
C	4.53542200	3.88552400	-0.74813100
H	5.76002000	3.24534900	0.90030500
H	3.21250500	4.20853300	-2.41911100
H	5.00813700	4.85912000	-0.82644200
C	2.97406400	-1.06531700	1.03858400
C	3.21433700	-2.44542600	1.03496900
C	3.00339400	-0.38194600	2.25955900

C	3.48494300	-3.12022100	2.22123900
H	3.19658600	-2.99387500	0.09663600
C	3.29179700	-1.05543300	3.44470700
H	2.79518000	0.68570700	2.29109400
C	3.53042000	-2.42655400	3.42923000
H	3.67062400	-4.18930400	2.19990300
H	3.32521300	-0.50372100	4.37940200
H	3.75696400	-2.95174200	4.35148200
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C	-3.17117600	-0.96141500	2.26320400
C	-2.95397800	1.41514400	1.92688800
C	-3.37477600	-0.74850700	3.62505200
H	-3.16408800	-1.97684300	1.87587400
C	-3.15592700	1.62589900	3.28752100
H	-2.76995700	2.26591600	1.27414700
C	-3.37467400	0.54469300	4.13938600
H	-3.53806200	-1.59737100	4.28177000
H	-3.14163200	2.63756400	3.68145100
H	-3.54287500	0.71141700	5.19847000
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C	-2.91926300	-2.43538100	-1.91115300
C	-4.67488000	-1.96421000	-0.31190400
C	-3.65411800	-3.52369200	-2.38052500
H	-1.97972000	-2.14650600	-2.37844200
C	-5.39868400	-3.05264900	-0.78445500
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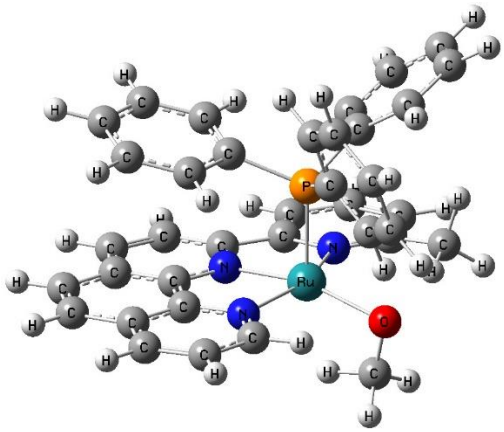
C	-4.88354000	-3.84114700	-1.81201900
H	-3.26574800	-4.11756500	-3.20229400
H	-6.36974400	-3.27956100	-0.35654100
H	-5.45108200	-4.69027700	-2.17922900
C	-3.31658600	1.10225400	-1.36535200
C	-2.90335700	1.13635800	-2.70295100
C	-4.35379700	1.93387000	-0.93961200
C	-3.49675700	2.02292200	-3.59490200
H	-2.12571400	0.44554300	-3.02592000
C	-4.93869200	2.82673100	-1.83655600
H	-4.72118800	1.88157900	0.08039400
C	-4.50687300	2.87897300	-3.15880700
H	-3.17574600	2.03991300	-4.63209800
H	-5.74297000	3.47366000	-1.50161800
H	-4.96878100	3.57329100	-3.85321800
C	-0.02660900	-3.65794000	-1.02147600
H	0.94034500	-4.12927700	-1.23432500
H	-0.80983400	-4.38200500	-1.26373200
H	-0.13779200	-2.77543100	-1.65460900

I2



SCF done	-2102.41777812
SCF done for solvent	-2102.46719722
Zero-point correction	0.595230
Thermal correction to Gibbs free energy	0.529357

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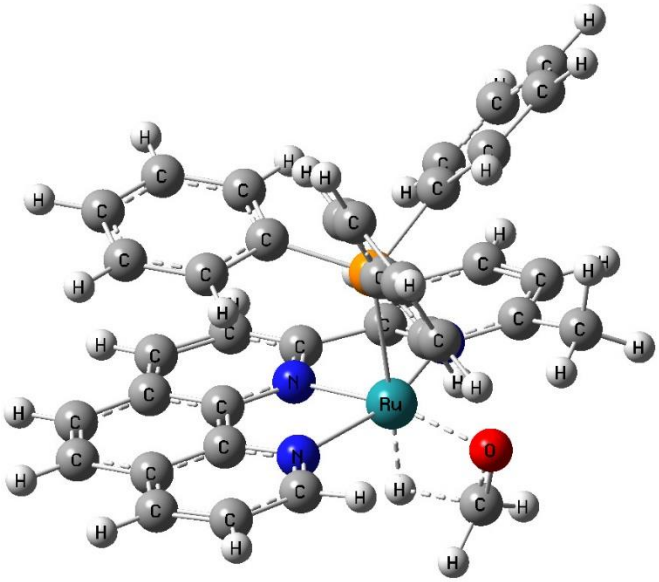
C	3.82265600	1.77449800	-1.83035700
C	4.80339200	-1.33138600	0.04771400
C	4.05926400	-0.31309900	-0.64927000
C	4.20031100	-2.44300200	0.55059400
C	2.44068500	1.52729200	-1.93738400
C	2.67420500	-0.47364200	-0.79969700
C	2.78520300	-2.64308000	0.39844300
C	2.04824800	-1.65154700	-0.26061300
C	2.05689800	-3.76892300	0.84993100
C	0.70010700	-3.87061000	0.61460700
C	0.03145900	-2.82226300	-0.05505800
C	-1.41326800	-2.75114000	-0.39912100
C	-3.12831100	-1.44487200	-1.31018400
C	-2.29510400	-3.77236800	-0.08198600
C	-4.05750600	-2.45807100	-1.02239400
C	-3.64278100	-3.62452600	-0.41023800
H	5.69802600	1.03304300	-1.09232300
H	4.23241300	2.68317000	-2.25485600
H	5.87433600	-1.19316100	0.16138100
H	4.78271000	-3.19956600	1.06670500
H	1.76166500	2.21537400	-2.43403800
H	2.57727800	-4.56649200	1.37113600
H	0.15900000	-4.74889500	0.94553500
H	-1.94389100	-4.67183400	0.40906700
H	-5.09952600	-2.29783700	-1.27680300
H	-4.35168300	-4.41308500	-0.18104800
N	1.88120400	0.43925000	-1.43220600

N	0.71814000	-1.75402300	-0.43643200
N	-1.82977700	-1.60671400	-1.02215000
Ru	-0.17833900	-0.20180700	-1.38259500
O	-0.84193800	1.19038200	-2.81136000
C	-0.59397300	0.26674700	-3.78583200
H	-1.49780400	-0.15325700	-4.25768000
H	0.10359300	0.60669200	-4.56668000
H	-0.05125100	-0.68165600	-3.37859300
P	-0.50948800	0.95792700	0.54986900
C	-2.21874300	0.91507300	1.22016600
C	-2.83257800	-0.29536200	1.57238600
C	-2.96949600	2.09466300	1.29506800
C	-4.15338500	-0.32309700	2.00562600
H	-2.29340100	-1.23353200	1.49149900
C	-4.29637200	2.06203400	1.71797100
H	-2.52532000	3.04369200	1.01542400
C	-4.89109200	0.85662800	2.07656200
H	-4.60792400	-1.27025000	2.27857100
H	-4.86373000	2.98543400	1.76589300
H	-5.92405800	0.83479300	2.40765600
C	-0.13152400	2.74040100	0.43607500
C	0.16396600	3.47816200	1.59128500
C	-0.23182000	3.38698700	-0.79996100
C	0.37800700	4.84865200	1.50457000
H	0.22748800	2.98076100	2.55545700
C	-0.01810100	4.76382000	-0.87491700
H	-0.48631400	2.81791600	-1.69201100
C	0.28960100	5.49189400	0.26984400
H	0.61011500	5.41590600	2.39976500
H	-0.10092800	5.26573600	-1.83358000
H	0.45469600	6.56257800	0.20534500
C	0.63359000	0.36457700	1.86457900
C	0.30092700	-0.67349900	2.73982100
C	1.95167800	0.84263100	1.85764600
C	1.26533900	-1.22945800	3.57779300
H	-0.71609500	-1.04388200	2.79494700
C	2.91113400	0.29299000	2.70306200
H	2.23152100	1.65289100	1.18793700
C	2.57246200	-0.75140200	3.55969700
H	0.98717400	-2.02967700	4.25612900
H	3.92472700	0.68132700	2.68811600
H	3.31991500	-1.18123500	4.21852200
C	-3.59045600	-0.13546500	-1.87446400
H	-2.76277800	0.45934800	-2.27331700
H	-4.34553700	-0.29825400	-2.64731100
H	-4.06390200	0.43616300	-1.06528000

TS1

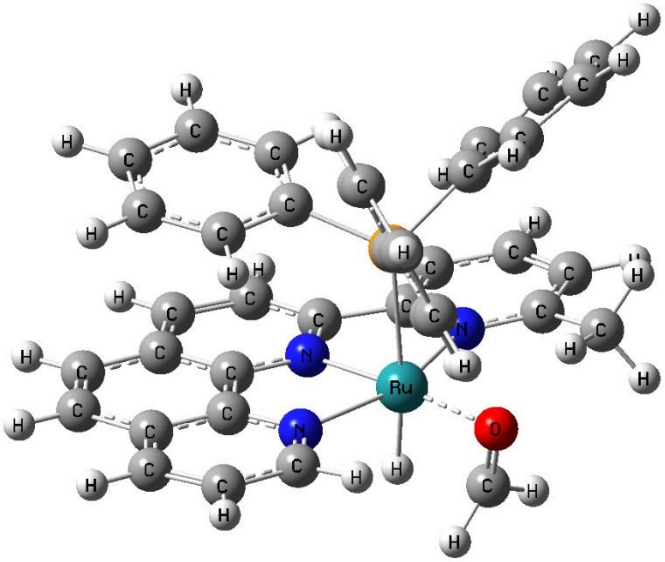


SCF done	-2102.40248280
SCF done for solvent	-2102.45056242
Zero-point correction	0.590562
Thermal correction to Gibbs free energy	0.523738

C	4.65636100	0.73720000	-1.11994400
C	3.88891000	1.61951300	-1.84951500
C	4.74638200	-1.38073300	0.24430800
C	4.04934300	-0.40290600	-0.55182900
C	4.10602300	-2.45220700	0.78573200
C	2.51477800	1.36825500	-2.02170700
C	2.67355200	-0.56842800	-0.77091800
C	2.69799900	-2.64875800	0.57811100
C	2.00813500	-1.70041200	-0.18688100
C	1.93478700	-3.73017600	1.07534700
C	0.58648200	-3.82556700	0.79600400
C	-0.03687400	-2.82005000	0.02557400
C	-1.47056400	-2.74017300	-0.35113500
C	-3.13924000	-1.44725900	-1.35129800
C	-2.38757800	-3.70167900	0.04569200
C	-4.10460300	-2.39728200	-0.98259200
C	-3.72993000	-3.53238800	-0.29021200
H	5.71861500	0.91118300	-0.97591700
H	4.32448000	2.50617600	-2.29437800
H	5.81125900	-1.24263600	0.40515300
H	4.65293700	-3.17753300	1.37974800

H	1.87242100	2.03827600	-2.58721400
H	2.42036100	-4.49564500	1.67281200
H	0.01575000	-4.66648200	1.17088500
H	-2.06746200	-4.56949500	0.60930800
H	-5.14230400	-2.21392700	-1.23924200
H	-4.46575000	-4.27463200	0.00050200
N	1.92145400	0.30533500	-1.50083800
N	0.68609400	-1.80062200	-0.41746000
N	-1.84412000	-1.63665100	-1.06691000
Ru	-0.13488500	-0.33037700	-1.51670900
O	-0.76178500	1.16167100	-2.98612800
C	-0.47840300	0.12735800	-3.68841600
H	-1.29412200	-0.50003100	-4.07400400
H	0.43675000	0.12478700	-4.29435700
H	0.18231600	-1.24692600	-2.82408200
P	-0.53000300	1.03885700	0.52479000
C	-2.23916600	1.07358700	1.20059900
C	-2.90919500	-0.12242700	1.49794700
C	-2.93750400	2.28057800	1.32222300
C	-4.23240300	-0.10892400	1.92674400
H	-2.40824800	-1.07912200	1.38483200
C	-4.26591100	2.28989500	1.74093600
H	-2.44852500	3.21923800	1.08514800
C	-4.91630400	1.09840100	2.04692600
H	-4.73003200	-1.04572000	2.15754500
H	-4.79100500	3.23527400	1.82849100
H	-5.95052000	1.10950400	2.37454900
C	-0.07018800	2.80241800	0.40261400
C	0.22721900	3.55837300	1.54515600
C	-0.08148800	3.41756500	-0.85251300
C	0.52092100	4.91181800	1.42744300
H	0.22700600	3.08652600	2.52421900
C	0.21070600	4.77723700	-0.96243600
H	-0.33094500	2.83634700	-1.73587100
C	0.51416000	5.52158500	0.17274700
H	0.75189400	5.49280400	2.31417400
H	0.19463600	5.25323200	-1.93761000
H	0.74118500	6.57912800	0.08457000
C	0.57075000	0.41653800	1.86185400
C	0.17960000	-0.58816900	2.75167100
C	1.91113600	0.83022800	1.86035400
C	1.10551400	-1.16709900	3.61758800
H	-0.85536100	-0.90891600	2.79536100
C	2.83245800	0.25488400	2.73045300
H	2.23504700	1.61481600	1.17954300
C	2.43372500	-0.75100800	3.60762400
H	0.78063000	-1.93669100	4.31069000
H	3.86322400	0.59567400	2.72253900
H	3.15136000	-1.19723000	4.28848400
C	-3.56710900	-0.16288600	-1.99591400
H	-2.73612400	0.37508700	-2.45406800
H	-4.34909600	-0.34429700	-2.73675600
H	-3.98999200	0.48373500	-1.21627800

I3



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SCF done for solvent	-2102.45191349
Zero-point correction	0.591999
Thermal correction to Gibbs free energy	0.524473

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C	3.90051600	1.53321000	-1.93925000
C	4.73595800	-1.39456100	0.26218900
C	4.04680600	-0.44547300	-0.57465000
C	4.08939500	-2.44393900	0.83813400
C	2.52717800	1.27809500	-2.11367800
C	2.67318300	-0.61752800	-0.80146100
C	2.68302900	-2.64533400	0.62614500
C	2.00126300	-1.72715600	-0.18183800
C	1.91239200	-3.70214600	1.16241300
C	0.56462500	-3.80322500	0.88269200
C	-0.05060400	-2.82627300	0.07052700
C	-1.48639200	-2.74854200	-0.30069800
C	-3.15394400	-1.47467700	-1.32186900
C	-2.40696100	-3.68528200	0.14282400
C	-4.12529600	-2.39892400	-0.90381300
C	-3.75300400	-3.51393900	-0.17980700
H	5.72194500	0.85156300	-1.02835500
H	4.34087500	2.40489000	-2.40833500
H	5.79951400	-1.25131700	0.42717000
H	4.62981000	-3.14654500	1.46455400
H	1.89039900	1.93407800	-2.70130800

H	2.39138800	-4.44318400	1.79513900
H	-0.01163500	-4.62320500	1.29339800
H	-2.08842200	-4.53441800	0.73489200
H	-5.16492300	-2.20945300	-1.14865900
H	-4.49198500	-4.23639500	0.14978000
N	1.92815800	0.23220200	-1.56650000
N	0.68099600	-1.83364600	-0.41415500
N	-1.85751900	-1.66806400	-1.05182300
Ru	-0.13196500	-0.39098700	-1.56504400
O	-0.81569200	1.21403700	-2.87055600
C	-0.59189000	0.20977000	-3.62551400
H	-1.43134400	-0.40315600	-3.97966600
H	0.31193500	0.18656700	-4.24630400
H	0.20305500	-1.43995000	-2.71190700
P	-0.51968300	1.07424000	0.50440800
C	-2.23850300	1.15461000	1.15150000
C	-2.94326300	-0.02209200	1.44546300
C	-2.91036800	2.37895700	1.24632300
C	-4.27439300	0.02788700	1.84763800
H	-2.46191500	-0.99141000	1.35510900
C	-4.24610800	2.42463200	1.63739700
H	-2.39391200	3.30321500	1.01079600
C	-4.93109700	1.25226400	1.94210700
H	-4.79858100	-0.89429500	2.07892900
H	-4.74992700	3.38311900	1.70557000
H	-5.97077500	1.29139900	2.24984800
C	-0.00346900	2.82586500	0.41470800
C	0.28191000	3.55947000	1.57506300
C	0.04797800	3.45474600	-0.83222900
C	0.62368800	4.90341900	1.48273200
H	0.23299700	3.07748000	2.54785600
C	0.38947300	4.80478600	-0.91719500
H	-0.19628200	2.89208700	-1.72806700
C	0.67936400	5.52650100	0.23566800
H	0.84352000	5.46714300	2.38336400
H	0.42296700	5.29125200	-1.88674700
H	0.94445900	6.57667400	0.16788200
C	0.54587000	0.41753000	1.85391500
C	0.11448200	-0.55649500	2.75865900
C	1.90062100	0.78400300	1.85377300
C	1.01457500	-1.14991000	3.64261600
H	-0.93182900	-0.83895800	2.80102900
C	2.79565700	0.19373300	2.74030000
H	2.25423200	1.54819300	1.16470500
C	2.35637900	-0.78085900	3.63409300
H	0.65826700	-1.89309600	4.34897600
H	3.83737000	0.49946300	2.73462400
H	3.05349400	-1.23751600	4.32925700
C	-3.57598800	-0.22764600	-2.03977800
H	-2.75340100	0.48237100	-2.14031600
H	-3.96361600	-0.47145500	-3.03441400
H	-4.38456200	0.25052100	-1.47806700

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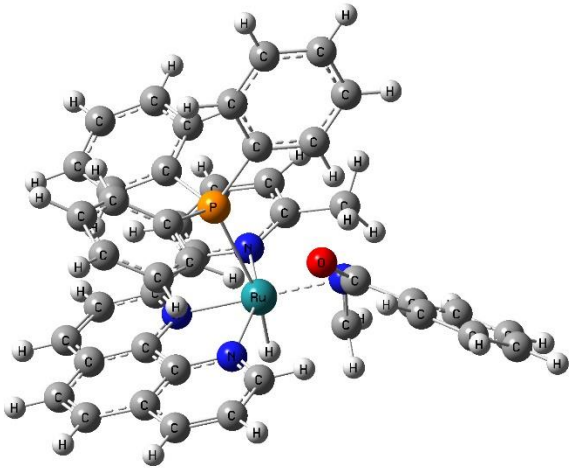


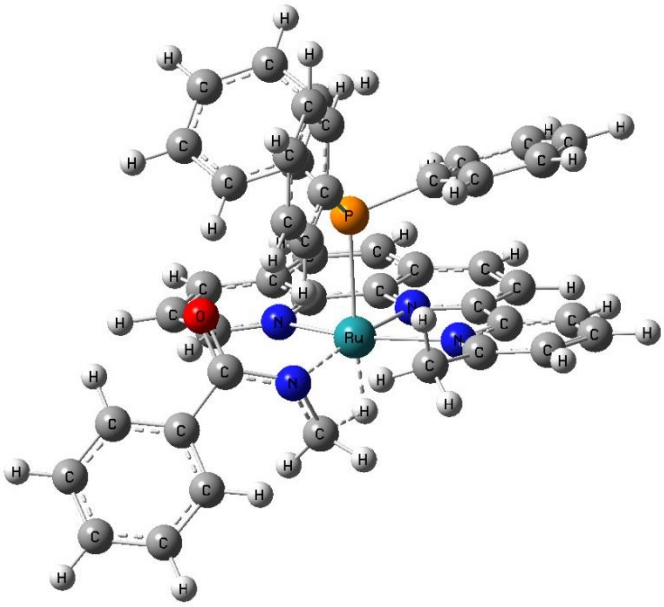
SCF done	-2426.79803430
SCF done for solvent	-2426.84824248
Zero-point correction	0.697554
Thermal correction to Gibbs free energy	0.621859

C	-0.82025600	4.80025600	-0.40110700
C	-1.96929700	4.04554200	-0.43696300
C	1.66686500	4.88748000	-0.71726500
C	0.41594800	4.17761500	-0.67180000
C	2.83011100	4.26523100	-1.04588000
C	-1.88713800	2.66718300	-0.70961400
C	0.39934300	2.79715600	-0.93207100
C	2.84436900	2.86153700	-1.34264000
C	1.64123200	2.14805200	-1.25179300
C	3.98362900	2.12632300	-1.74947600
C	3.89073200	0.77916700	-2.01920600
C	2.64821900	0.12297000	-1.86008500
C	2.39928400	-1.33040100	-2.02431300
C	0.85192700	-3.06585500	-1.97029100
C	3.44091100	-2.20394700	-2.29650400
C	1.86932600	-3.99260400	-2.24487300
C	3.17048300	-3.56475200	-2.40894900
H	-0.85341700	5.86396400	-0.18538300
H	-2.94148300	4.48824900	-0.25561200
H	1.65753300	5.95050600	-0.49783900
H	3.76066700	4.82131300	-1.09583700
H	-2.78609600	2.06113100	-0.72051600
H	4.93587300	2.63722500	-1.85578900
H	4.76828500	0.22909700	-2.33473000

H	4.45376200	-1.83612000	-2.39787700
H	1.61045600	-5.04295900	-2.32202800
H	3.96834700	-4.27032000	-2.61410700
N	-0.74091200	2.04346700	-0.93212800
N	1.58732600	0.82406700	-1.49481800
N	1.11222400	-1.75632100	-1.85676700
Ru	-0.24217600	-0.05716100	-1.29600600
H	-0.29218200	0.29650500	-2.82451900
P	0.48097900	-0.44743800	1.24166400
C	-0.37769400	-1.62505700	2.35008600
C	-1.31270600	-2.51774900	1.82389600
C	-0.04732500	-1.68667900	3.70770300
C	-1.90474900	-3.47348100	2.64720600
H	-1.58579400	-2.44864900	0.77589700
C	-0.64570400	-2.63616200	4.52753300
H	0.67368100	-0.98856200	4.12384000
C	-1.57232300	-3.53284300	3.99691800
H	-2.63366000	-4.16386200	2.23533500
H	-0.39054300	-2.67655300	5.58136500
H	-2.03799700	-4.27310300	4.63940400
C	0.63471600	1.07571500	2.26458600
C	1.72758700	1.37072400	3.08854600
C	-0.45039700	1.96161600	2.23447100
C	1.75262600	2.55063100	3.82886700
H	2.55967600	0.67880500	3.16681900
C	-0.42032400	3.13927200	2.97484300
H	-1.33012400	1.69547700	1.65944900
C	0.68688100	3.44341100	3.76318100
H	2.60514400	2.76651100	4.46470400
H	-1.27141300	3.81287800	2.94553100
H	0.71042700	4.36110500	4.34188000
C	2.17895200	-1.16242200	1.20882100
C	2.33670600	-2.55509100	1.23938400
C	3.31244900	-0.36716700	1.00166100
C	3.59308900	-3.13091700	1.08021400
H	1.47162100	-3.19301900	1.40104000
C	4.57307200	-0.94412500	0.85765800
H	3.21442200	0.71547400	0.95129800
C	4.71724800	-2.32756000	0.89561600
H	3.69563300	-4.21107500	1.11258900
H	5.44117800	-0.30649900	0.71733900
H	5.69900600	-2.77789500	0.78916100
N	-2.18799100	-0.92565900	-1.00158900
C	-3.07610100	-0.32581700	-0.12439900
C	-4.52579500	-0.35083400	-0.50615500
C	-5.39947700	0.43410300	0.25360900
C	-5.02527200	-1.11449000	-1.56539700
C	-6.75281900	0.47418400	-0.05690900
H	-4.99432100	0.99620100	1.08875800
C	-6.38213100	-1.07825900	-1.86910500
H	-4.36281500	-1.75654000	-2.13669300
C	-7.24462900	-0.28050900	-1.12070400
H	-7.42591800	1.08749900	0.53274500
H	-6.76833300	-1.67857100	-2.68602300
H	-8.30235500	-0.25374300	-1.36164800
C	-0.55746000	-3.55694800	-1.82498400

H	-0.98521300	-3.74536800	-2.81619500
H	-0.57154900	-4.50410000	-1.28040100
H	-1.18661300	-2.83459300	-1.30497000
C	-2.07234100	-0.59056300	-2.29906600
H	-1.85030100	-1.38021100	-3.01629800
O	-2.71520300	0.15740700	0.93858600
H	-2.61803700	0.26472300	-2.70443100

$TS2_N$



SCF done	-2426.79632758
SCF done for solvent	-2426.84644291
Zero-point correction	0.696321
Thermal correction to Gibbs free energy	0.621321

C	-0.80857000	4.80690600	-0.11659800
C	-1.93379400	4.03660100	0.04904100
C	1.58684100	4.92558300	-0.83961300
C	0.37356200	4.19598500	-0.58406300
C	2.69093600	4.31858600	-1.34943700
C	-1.87867000	2.65644500	-0.22269000
C	0.33421500	2.81268400	-0.83109400
C	2.67968100	2.91250400	-1.63160700
C	1.51929100	2.17966700	-1.34152400
C	3.75427400	2.19402600	-2.20679700
C	3.64327600	0.84346900	-2.44824600
C	2.45424900	0.16875300	-2.08812000
C	2.21478400	-1.29003200	-2.19694300

C	0.76712100	-3.06793900	-1.79734500
C	3.21070600	-2.14191700	-2.64984700
C	1.73801400	-3.97106600	-2.25783100
C	2.96398400	-3.51074100	-2.69184000
H	-0.81906900	5.87224700	0.09321500
H	-2.86672600	4.46518500	0.39547800
H	1.59400900	5.99061700	-0.62997300
H	3.59121600	4.88755000	-1.55763700
H	-2.74948700	2.03402400	-0.05648500
H	4.66756800	2.72116900	-2.46543900
H	4.46912700	0.30675900	-2.89761200
H	4.17149900	-1.75059600	-2.95819700
H	1.50473900	-5.03019000	-2.25692100
H	3.72373600	-4.19766700	-3.04860600
N	-0.78095400	2.04456000	-0.64091700
N	1.45198400	0.85101200	-1.55667100
N	0.99234900	-1.74606100	-1.78818900
Ru	-0.30579100	-0.07246900	-1.08200800
H	-0.71224500	0.25818200	-2.60247500
P	0.63980500	-0.46104600	1.24298900
C	-0.08416500	-1.71113100	2.36440500
C	-1.21405000	-2.43827000	1.99080800
C	0.51339300	-1.94061200	3.61060900
C	-1.73514300	-3.40229900	2.85468700
H	-1.68526500	-2.24100800	1.03390100
C	-0.00965400	-2.89996600	4.46706100
H	1.38669200	-1.36495700	3.90731600
C	-1.13449500	-3.63379400	4.08710200
H	-2.61723200	-3.96400300	2.56516900
H	0.45415800	-3.07345900	5.43241700
H	-1.54425800	-4.38050300	4.75947400
C	0.72449800	1.02840400	2.31242400
C	1.86699800	1.47944800	2.97971300
C	-0.48931600	1.70572200	2.49357100
C	1.80657400	2.62176900	3.77592300
H	2.80382200	0.93851400	2.89935300
C	-0.54243600	2.84446600	3.29029600
H	-1.39232300	1.31102900	2.03246900
C	0.60798700	3.31299900	3.92197400
H	2.69867400	2.96302000	4.29114000
H	-1.48877900	3.35821900	3.42884400
H	0.56634400	4.20127900	4.54394300
C	2.36889300	-1.05564400	1.05900600
C	2.62995200	-2.43315100	1.07035600
C	3.41215100	-0.18016200	0.73390900
C	3.90049800	-2.91675300	0.77504600
H	1.83541900	-3.13132100	1.32037400
C	4.68874700	-0.66455200	0.45552600
H	3.22939800	0.89176300	0.69216200
C	4.93579400	-2.03398800	0.47244600
H	4.08428300	-3.98634000	0.79139100
H	5.48779500	0.03322300	0.22364100
H	5.93032900	-2.41242100	0.25900100
N	-2.26705300	-0.93360900	-0.86239400
C	-3.23444400	-0.37881400	-0.05286700
C	-4.64714500	-0.39636500	-0.55813900

C	-5.57498500	0.42363000	0.09086900
C	-5.06197200	-1.19725600	-1.62627600
C	-6.89332800	0.46882600	-0.34510300
H	-5.24344300	1.00972000	0.94189500
C	-6.38495100	-1.15909900	-2.05417000
H	-4.35971800	-1.87298900	-2.10434100
C	-7.29849300	-0.32052400	-1.42034300
H	-7.60843500	1.11302600	0.15557500
H	-6.70463900	-1.78855700	-2.87779800
H	-8.32920600	-0.28898000	-1.75818800
C	-0.52186700	-3.61176500	-1.25764900
H	-0.86598300	-4.44888400	-1.86940300
H	-0.34954300	-3.99346000	-0.24398300
H	-1.30080700	-2.85378100	-1.18736200
C	-2.11842500	-0.62297400	-2.17628300
H	-1.86908100	-1.43570600	-2.86105700
O	-2.97467600	0.06794500	1.05838500
H	-2.73478400	0.16276900	-2.61971700

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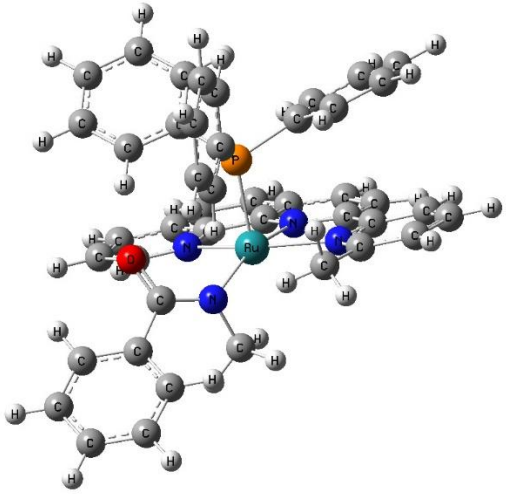

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SCF done for solvent	-2426.87666652
Zero-point correction	0.700986
Thermal correction to Gibbs free energy	0.626263

C	-0.02819600	4.93395300	-0.17064100
C	-1.20702800	4.29370200	0.12717400
C	2.32355400	4.75465100	-1.03801600
C	1.05896200	4.17907900	-0.66303400
C	3.32897400	3.99839400	-1.55514200
C	-1.31266000	2.89963000	-0.05298600
C	0.86664600	2.79643100	-0.80857300

C	3.15837400	2.58465400	-1.73224300
C	1.94479200	2.00492800	-1.33558700
C	4.11607900	1.71223800	-2.30328900
C	3.83861100	0.37159900	-2.45895700
C	2.59887300	-0.13730200	-2.00954300
C	2.16059400	-1.55455100	-2.06851200
C	0.43699900	-3.08472800	-1.73044300
C	3.03321200	-2.55391800	-2.46838700
C	1.27982200	-4.13328900	-2.13255600
C	2.58383800	-3.87206200	-2.49863600
H	0.07691200	6.00686100	-0.03937100
H	-2.06364100	4.83905900	0.50525800
H	2.45444600	5.82486900	-0.91098800
H	4.26920200	4.45382600	-1.84911100
H	-2.21678200	2.35682400	0.20919300
H	5.06822200	2.11274400	-2.63790600
H	4.56847900	-0.28147700	-2.92075100
H	4.05466100	-2.31671200	-2.73760400
H	0.88521700	-5.14345900	-2.14476100
H	3.24802700	-4.67351800	-2.80382600
N	-0.30821500	2.16558500	-0.50786700
N	1.71645400	0.68138200	-1.45824600
N	0.87162700	-1.81693300	-1.69459600
Ru	-0.14709900	0.03675500	-0.91268400
H	-1.30102700	0.28753000	-2.81484600
P	0.52023500	-0.48075500	1.20427800
C	-0.46690100	-1.67483800	2.17476300
C	-1.69296400	-2.15717200	1.72265000
C	0.01596100	-2.06434100	3.43262700
C	-2.42549400	-3.04191700	2.51423600
H	-2.07588000	-1.83132700	0.76459600
C	-0.71589700	-2.94698200	4.21508000
H	0.96262700	-1.67308700	3.79788100
C	-1.93891200	-3.43789200	3.75399600
H	-3.38410200	-3.40750300	2.16138500
H	-0.33940600	-3.24705500	5.18725400
H	-2.51383200	-4.12144200	4.37027500
C	0.64612700	0.92526700	2.37359900
C	1.80408900	1.29083700	3.06551400
C	-0.55669500	1.59866000	2.63129100
C	1.76982100	2.35287400	3.96824700
H	2.72981600	0.74287000	2.93284300
C	-0.58058800	2.65527900	3.53450100
H	-1.47152300	1.27010000	2.13910500
C	0.58394000	3.04294000	4.19504600
H	2.67229100	2.62916600	4.50356900
H	-1.51685000	3.16713000	3.73405200
H	0.56126300	3.86664100	4.90126100
C	2.18262900	-1.26553400	1.13985100
C	2.30240100	-2.65982500	1.19472500
C	3.32925600	-0.50288500	0.88351000
C	3.53880400	-3.27225700	1.00796800
H	1.42700400	-3.27146700	1.39395600
C	4.56772900	-1.11531200	0.71067500
H	3.25755500	0.57983900	0.80648000
C	4.67499300	-2.50230000	0.77054600

H	3.61383900	-4.35384900	1.05722900
H	5.44683500	-0.50590100	0.52515600
H	5.64029300	-2.98019600	0.63831900
N	-2.21539900	-0.34928800	-1.02836500
C	-3.22311000	0.09924300	-0.25576500
C	-4.63335500	0.07646800	-0.78299700
C	-5.53393000	1.02119900	-0.28612900
C	-5.08252200	-0.89195400	-1.68386700
C	-6.85588300	1.02420400	-0.71516700
H	-5.18048300	1.73576200	0.45001300
C	-6.41013400	-0.90044900	-2.10106900
H	-4.39643900	-1.65581200	-2.03991500
C	-7.29493700	0.06423600	-1.62506200
H	-7.54893700	1.76634900	-0.33275300
H	-6.75666400	-1.66216400	-2.79181900
H	-8.32896800	0.06082000	-1.95425900
C	-0.96604500	-3.40081300	-1.30805300
H	-1.41055200	-4.12304700	-1.99741100
H	-0.95531100	-3.85724100	-0.31173000
H	-1.58399000	-2.50408900	-1.25591400
C	-2.23832600	-0.23891400	-2.46929800
H	-2.23227300	-1.20536100	-2.98981800
O	-3.03465000	0.49241100	0.90744400
H	-3.05429300	0.37650500	-2.85945100

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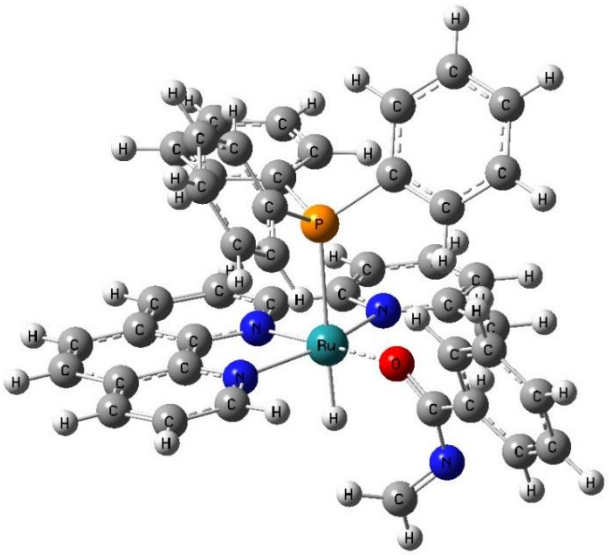
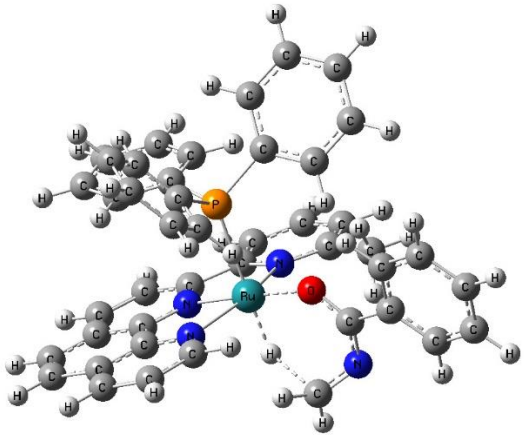


SCF done	-2426.79434450
SCF done for solvent	-2426.84205023
Zero-point correction	0.695044
Thermal correction to Gibbs free energy	0.615729

C	1.35665500	4.87695000	-0.29997600
C	0.00593400	4.61308500	-0.33932400
C	3.69797600	3.99227700	-0.53535600
C	2.26809000	3.82630000	-0.53363100
C	4.53499500	2.95210800	-0.79289800
C	-0.43482900	3.30185200	-0.59253500
C	1.73205100	2.55243800	-0.78820500
C	4.01667400	1.64263700	-1.07543800
C	2.62644200	1.46501000	-1.06574200
C	4.80201800	0.50413400	-1.36305200
C	4.19675500	-0.70754000	-1.61610100
C	2.78966600	-0.80534500	-1.59237900
C	1.98955800	-2.02020000	-1.85971200
C	-0.15130900	-2.91478000	-2.06051200
C	2.57767300	-3.24055400	-2.17553900
C	0.38473200	-4.16653600	-2.37315600
C	1.76029900	-4.33433800	-2.42471400
H	1.72639600	5.87805300	-0.09968100
H	-0.72536100	5.39538800	-0.17417400
H	4.09860100	4.98024900	-0.33040200
H	5.61050400	3.09852300	-0.79550300
H	-1.49505200	3.06323100	-0.61657000
H	5.88402500	0.59003000	-1.37979100
H	4.80126200	-1.58051300	-1.82926900
H	3.65553300	-3.33586900	-2.22005800
H	-0.28659700	-4.99221500	-2.57921900
H	2.19136800	-5.29995400	-2.66659500
N	0.39223300	2.28948500	-0.80233600
N	2.05362800	0.26892500	-1.31957200
N	0.64187300	-1.86537000	-1.78561900
Ru	0.06606500	0.18160900	-1.20298100
P	0.19896600	-0.52245900	1.28520200
C	-0.86520800	-1.85290100	1.97636000
C	-2.18195000	-1.92435500	1.51074900
C	-0.45907500	-2.70378400	3.01000200
C	-3.07525300	-2.84450900	2.05482500
H	-2.50922100	-1.24609300	0.72680400
C	-1.35022500	-3.62861100	3.54566100
H	0.55420200	-2.64537100	3.39711700
C	-2.65755700	-3.70238500	3.06778100
H	-4.09532400	-2.88770500	1.68607300
H	-1.02537100	-4.28838700	4.34363700
H	-3.34965900	-4.42350100	3.49009400
C	-0.03401700	0.78100200	2.55666000
C	0.60139600	0.77543700	3.80231500
C	-0.97551200	1.77415900	2.27319500
C	0.31650400	1.76597900	4.73618300
H	1.32129500	-0.00297700	4.04014300
C	-1.26628300	2.76171600	3.21151000
H	-1.48598000	1.75397100	1.31268800
C	-0.61353300	2.76177600	4.44085800
H	0.81598300	1.75812200	5.69956800
H	-2.00033900	3.52891200	2.98478400

H	-0.83238900	3.53204500	5.17321800
C	1.91015900	-1.12073300	1.55073600
C	2.24480500	-2.45148000	1.27207200
C	2.94079200	-0.21227600	1.83045700
C	3.57312800	-2.87192000	1.30928100
H	1.46289300	-3.16651800	1.02487900
C	4.26645600	-0.63309700	1.86228700
H	2.70453500	0.82938000	2.03531000
C	4.58661500	-1.96585200	1.60822300
H	3.81143200	-3.91119000	1.10459700
H	5.05109700	0.08261400	2.08832300
H	5.62012300	-2.29508100	1.64449600
C	-1.62930100	-2.68031400	-2.04282400
H	-1.94499100	-2.34982000	-1.05023400
H	-1.88595600	-1.89069700	-2.75652700
H	-2.17329500	-3.58885100	-2.30388200
C	-3.14531100	0.44203400	-1.67361000
O	-2.16191800	0.31362400	-0.93633100
C	-4.50639700	0.56346700	-1.11230000
C	-4.65288000	0.72698300	0.27098500
C	-5.63220800	0.52468600	-1.94174800
C	-5.92212100	0.84931500	0.81926200
H	-3.76953500	0.75712400	0.90169300
C	-6.90005600	0.64770100	-1.38534400
H	-5.50690500	0.38334500	-3.00986700
C	-7.04431100	0.80993100	-0.00897000
H	-6.04022300	0.97631800	1.88999300
H	-7.77619300	0.61350700	-2.02345600
H	-8.03567300	0.90536400	0.42199100
N	-3.02564000	0.37996600	-3.05225300
C	-2.26923000	1.19728300	-3.66034100
H	-1.78422300	2.04215800	-3.16389700
H	-2.10174800	1.07145100	-4.72862900
H	0.00730100	0.53053000	-2.75135900

TS2o

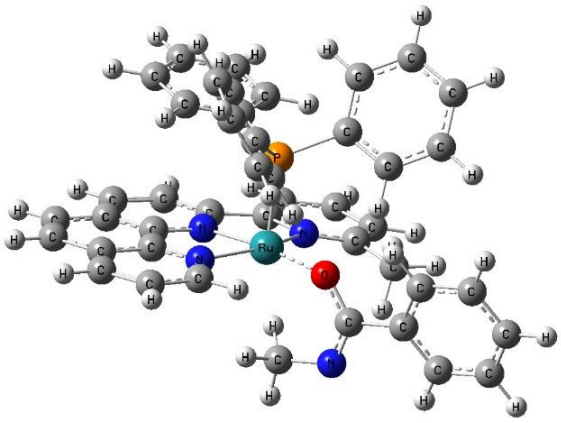


SCF done	-2426.79162809
SCF done for solvent	-2426.83905056
Zero-point correction	0.695945
Thermal correction to Gibbs free energy	0.620969

C	1.64272900	4.78971300	-0.34715500
C	0.28269600	4.61245900	-0.23501500
C	3.88479800	3.76150600	-0.82936900
C	2.45599400	3.68355100	-0.67238400
C	4.62469700	2.67053900	-1.16233700
C	-0.26633200	3.33202700	-0.43316600
C	1.81709700	2.44633700	-0.85908900
C	3.99980100	1.39406900	-1.36992700
C	2.60949700	1.30292300	-1.21421700
C	4.67976400	0.20545000	-1.71778900
C	3.98017900	-0.96972300	-1.88647500
C	2.57924900	-0.97857400	-1.71734900
C	1.68044600	-2.14080200	-1.89583300
C	-0.52591400	-2.88649400	-1.93088700
C	2.15963800	-3.39721800	-2.24964200
C	-0.09930100	-4.17184700	-2.27822400
C	1.25339400	-4.43378200	-2.42930300
H	2.09451200	5.76521000	-0.19467500
H	-0.37421300	5.43908200	0.00820400
H	4.36349300	4.72407500	-0.67886500
H	5.70075900	2.74980700	-1.28085700
H	-1.33596400	3.16113600	-0.34391300
H	5.75746800	0.22380800	-1.84725200
H	4.50638100	-1.88013800	-2.14495400
H	3.22190400	-3.56420300	-2.37860900
H	-0.83930000	-4.94824600	-2.43386400
H	1.59827200	-5.42618500	-2.69888800
N	0.46839700	2.27127100	-0.73021800
N	1.94443600	0.14240600	-1.39139200
N	0.35618900	-1.89696000	-1.71215800
Ru	-0.03156700	0.18622600	-1.08433300
P	0.28741700	-0.46713400	1.32310200
C	-0.81609600	-1.70793600	2.10742600
C	-2.15731500	-1.72082600	1.71330100
C	-0.40008800	-2.53876300	3.15376300
C	-3.06717400	-2.57037800	2.33882200
H	-2.48686200	-1.05111700	0.92384300
C	-1.30935000	-3.39150300	3.77111200
H	0.63401000	-2.51991300	3.48632400
C	-2.64214500	-3.41186100	3.36226000
H	-4.10636700	-2.57077000	2.02428700
H	-0.97898900	-4.03693500	4.57843100
H	-3.34762300	-4.07833300	3.84765800
C	0.21575900	0.87941600	2.56831900
C	1.01898900	0.93274400	3.71135000
C	-0.78601900	1.83887600	2.38863800

C	0.84619300	1.95549800	4.63939300
H	1.77734800	0.17426300	3.88165300
C	-0.96392100	2.85535300	3.32336300
H	-1.43793500	1.76549900	1.51992400
C	-0.13985400	2.92025500	4.44407000
H	1.47566900	1.99256100	5.52243100
H	-1.74664100	3.59377000	3.18015100
H	-0.27371300	3.71332300	5.17230800
C	1.96387700	-1.18862100	1.47282700
C	2.15861600	-2.55156100	1.21899000
C	3.08817500	-0.36470700	1.62439800
C	3.44466900	-3.08413400	1.15121100
H	1.30039800	-3.20373700	1.07301000
C	4.37132500	-0.89856300	1.55518900
H	2.96013800	0.70032300	1.80325700
C	4.55345900	-2.26094500	1.32307000
H	3.57574700	-4.14576300	0.96599500
H	5.23053900	-0.24730400	1.68396800
H	5.55473200	-2.67719300	1.27839400
C	-1.98019600	-2.55031800	-1.82710900
H	-2.22005500	-2.20777600	-0.81813700
H	-2.21869600	-1.73893400	-2.52293600
H	-2.59779500	-3.41748800	-2.06386500
C	-3.11965700	0.63639200	-1.53390400
O	-2.21368300	0.44200100	-0.69263400
C	-4.53365600	0.69179100	-1.10446000
C	-4.83918800	0.68670100	0.26158100
C	-5.55810400	0.75201900	-2.05425500
C	-6.16490600	0.73804400	0.67175800
H	-4.03272100	0.64828600	0.98772600
C	-6.88279400	0.80168100	-1.63756200
H	-5.30515400	0.74589700	-3.10892100
C	-7.18566900	0.79370300	-0.27728900
H	-6.40565700	0.73636300	1.72950800
H	-7.67986200	0.84377300	-2.37197800
H	-8.22104700	0.83107500	0.04570400
N	-2.84599200	0.68153800	-2.86405700
C	-1.81931900	1.34607300	-3.27500300
H	-1.42809200	2.20791800	-2.72944100
H	-1.49318900	1.22507800	-4.30572600
H	-0.21982200	0.51066500	-2.67852300

$I5_O$

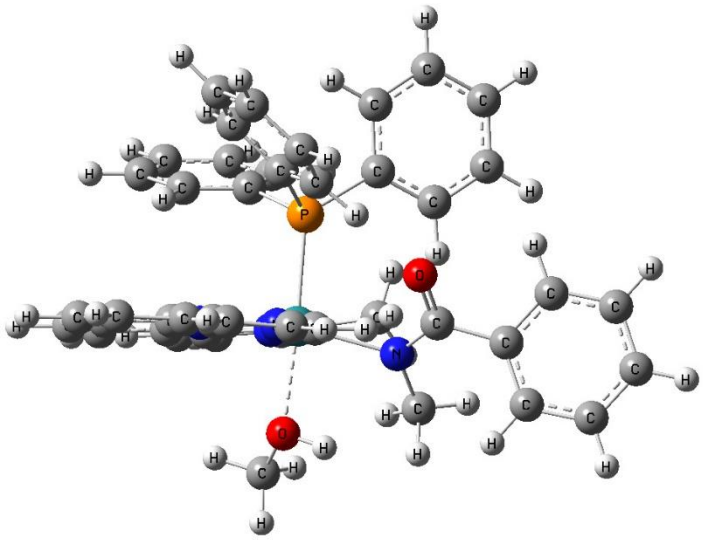


SCF done	-2426.82901337
SCF done for solvent	-2426.88299806
Zero-point correction	0.699999
Thermal correction to Gibbs free energy	0.624439

C	-2.43317600	-4.37089000	-1.10203600
C	-1.06788800	-4.45314100	-0.94830100
C	-4.45329100	-2.90096500	-1.42947400
C	-3.04170600	-3.10224900	-1.22888900
C	-4.98252200	-1.65668300	-1.58141900
C	-0.30222200	-3.27202000	-0.89328200
C	-2.19928300	-1.98200500	-1.16811300
C	-4.14182300	-0.49252300	-1.54870700
C	-2.76782400	-0.67330600	-1.34198000
C	-4.58456500	0.84196700	-1.69949600
C	-3.68775700	1.88848400	-1.65027200
C	-2.31571300	1.61936300	-1.45085200
C	-1.21213900	2.61258900	-1.42083000
C	1.09981900	2.93726500	-1.35549700
C	-1.44724300	3.97188300	-1.57180600
C	0.91591100	4.31956600	-1.49466800
C	-0.36160900	4.84227700	-1.58888900
H	-3.04468700	-5.26740900	-1.13923700
H	-0.56883500	-5.41126500	-0.86584300
H	-5.09441200	-3.77617200	-1.46416400
H	-6.04867300	-1.52688500	-1.73783400
H	0.77850700	-3.28727200	-0.78343400
H	-5.64093900	1.03908800	-1.85508100
H	-4.03879000	2.90643000	-1.76512300
H	-2.45742200	4.34858100	-1.67472500
H	1.78737100	4.96241400	-1.53653100
H	-0.51615600	5.91070400	-1.69537700
N	-0.85112000	-2.07201100	-0.97821600
N	-1.91092600	0.36642600	-1.30076300
N	0.04537000	2.10780900	-1.27508800
Ru	0.02822600	-0.10513500	-0.94532200

P	-0.27726500	0.17748400	1.31277800
C	1.02380900	1.09314700	2.21572300
C	2.35173000	0.89838500	1.82600800
C	0.74228200	1.81795800	3.38042800
C	3.38780700	1.46224600	2.56587900
H	2.56956800	0.28325500	0.95771700
C	1.78189200	2.38280800	4.11206400
H	-0.28070800	1.93647300	3.72428700
C	3.10365500	2.21314800	3.70271800
H	4.41378600	1.30052900	2.24860600
H	1.55833200	2.94934300	5.00996900
H	3.90937200	2.65547700	4.27954600
C	-0.32889400	-1.38676000	2.25652700
C	-1.17053300	-1.60793000	3.34970500
C	0.64225500	-2.33822400	1.92132000
C	-1.07707200	-2.79865300	4.06649900
H	-1.88962900	-0.85405100	3.65505200
C	0.73438500	-3.52178700	2.64678800
H	1.33427000	-2.13023800	1.10544100
C	-0.13395300	-3.75851100	3.71071900
H	-1.73653100	-2.97023900	4.91085200
H	1.49143500	-4.25562200	2.38811600
H	-0.06328000	-4.68304900	4.27434000
C	-1.83675500	1.07320100	1.64436000
C	-1.84529000	2.47296500	1.66776600
C	-3.05809200	0.38718000	1.67355600
C	-3.04837800	3.17072200	1.75185100
H	-0.90865400	3.02282300	1.62154500
C	-4.25808500	1.08663900	1.75604000
H	-3.07267900	-0.69944600	1.63506900
C	-4.25564000	2.47986200	1.80039900
H	-3.03755700	4.25557300	1.78330500
H	-5.19602900	0.54096000	1.78747700
H	-5.19213100	3.02315600	1.87466900
C	2.46943100	2.33775500	-1.35957700
H	2.59452900	1.64304400	-0.52909400
H	2.61939600	1.76268800	-2.28138900
H	3.23512800	3.11161600	-1.29918900
C	2.86302100	-0.82710500	-1.70212500
O	2.00161700	-0.87224300	-0.71154900
C	4.30261300	-0.83085300	-1.28591400
C	4.66012100	-1.15159900	0.02657400
C	5.30090900	-0.49150000	-2.20352800
C	5.99573800	-1.12329400	0.41986100
H	3.88655900	-1.43743400	0.73241600
C	6.63262800	-0.45607200	-1.80737300
H	5.00914900	-0.25869900	-3.22169300
C	6.98378300	-0.76934000	-0.49488100
H	6.26468500	-1.38369900	1.43896300
H	7.40157400	-0.18553500	-2.52398100
H	8.02479500	-0.74360000	-0.18897500
N	2.59783700	-0.74151200	-2.96087800
C	1.21924800	-0.79557600	-3.35902800
H	0.74474200	-1.76292500	-3.14247500
H	1.12750600	-0.62215200	-4.43426400
H	0.57487000	0.02964100	-2.93655200

I6



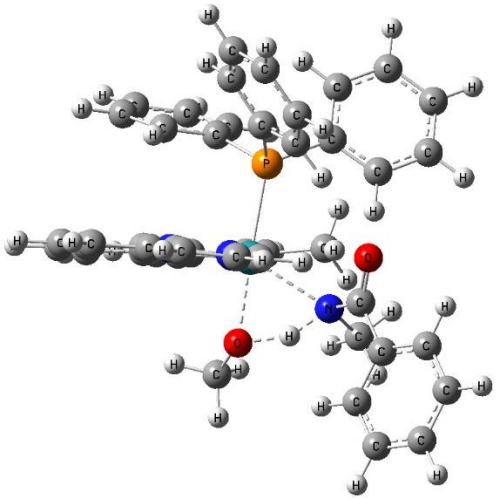
SCF done	-2542.52580067
SCF done for solvent	-2542.57930794
Zero-point correction	0.756090
Thermal correction to Gibbs free energy	0.676760

C	0.88907500	4.91446100	-0.26988600
C	-0.42501600	4.51679800	-0.32001400
C	3.30612900	4.27027100	-0.46909800
C	1.90372900	3.94994500	-0.44911200
C	4.25034900	3.32548400	-0.72154600
C	-0.73808800	3.15782400	-0.52367600
C	1.49970200	2.62001800	-0.64789200
C	3.86862100	1.96349100	-0.96152000
C	2.50933300	1.62458900	-0.88456500
C	4.76164100	0.92108200	-1.30259100
C	4.28895400	-0.34620600	-1.56221100
C	2.90686700	-0.61276200	-1.43358900
C	2.25758900	-1.93341500	-1.62635800
C	0.29470700	-3.17396600	-1.53156900
C	3.00856800	-3.06261300	-1.91896500
C	1.00231300	-4.34397500	-1.84338800
C	2.36577900	-4.29031800	-2.04975600
H	1.15617600	5.95415500	-0.10529400
H	-1.23333400	5.22743600	-0.19492700
H	3.59589800	5.30201500	-0.29535500
H	5.30267000	3.58837000	-0.75582600
H	-1.76298800	2.80409000	-0.50657400
H	5.82368800	1.13344000	-1.37962900
H	4.97847500	-1.13007600	-1.84881900

H	4.08314300	-2.99525200	-2.03106500
H	0.46056300	-5.28198500	-1.90141500
H	2.93065000	-5.18532900	-2.28690500
N	0.19267500	2.22786000	-0.67360300
N	2.07972800	0.35975700	-1.07537100
N	0.90242600	-1.98003000	-1.46563600
Ru	0.06410300	0.07847700	-1.00691600
H	-1.75496400	-1.39814300	-2.94347400
P	0.11909400	-0.39607500	1.29670100
C	-1.23331500	-1.23238100	2.21622300
C	-2.40254000	-1.68240100	1.60437100
C	-1.04820000	-1.45762800	3.58652700
C	-3.36863400	-2.35931300	2.34763700
H	-2.57096900	-1.49218700	0.55234100
C	-2.01323000	-2.12975900	4.32651100
H	-0.14574800	-1.10246500	4.07764400
C	-3.17606900	-2.58440800	3.70643300
H	-4.27748200	-2.69812600	1.85977500
H	-1.85958500	-2.29531900	5.38764800
H	-3.93133400	-3.10745100	4.28394300
C	0.49685000	1.02641400	2.40769500
C	-0.40519200	2.10000000	2.40648600
C	1.57553300	1.04989200	3.29906300
C	-0.18891400	3.19708600	3.23409600
H	-1.28917000	2.04757400	1.77914100
C	1.78431400	2.15127200	4.12669000
H	2.24853100	0.20483400	3.37865400
C	0.91291800	3.23374400	4.08595600
H	-0.89683700	4.02021200	3.22396400
H	2.62591600	2.15211600	4.81170000
H	1.07721200	4.08993000	4.73237800
C	1.50999600	-1.58412800	1.56601500
C	1.23546500	-2.95251600	1.68122100
C	2.84987800	-1.17981000	1.49764000
C	2.26731000	-3.88655400	1.72100200
H	0.20569100	-3.29275100	1.74865200
C	3.88316700	-2.11135200	1.56134000
H	3.09591300	-0.12576500	1.39347700
C	3.59479000	-3.46916600	1.66711200
H	2.03168800	-4.94236300	1.80990400
H	4.91380200	-1.77130900	1.52598500
H	4.39859200	-4.19659200	1.71773200
N	-2.07289300	-0.01210700	-1.41458500
C	-2.95532200	0.57058800	-0.59193600
C	-4.44007600	0.55232100	-0.86891100
C	-5.27324400	0.21442800	0.20187900
C	-5.01350500	0.92812100	-2.08527400
C	-6.65438700	0.20559700	0.04357600
H	-4.81734500	-0.02262500	1.15876600
C	-6.39772000	0.94560100	-2.23579200
H	-4.38413500	1.23306000	-2.91570300
C	-7.21952500	0.57115400	-1.17664500
H	-7.29229900	-0.07069700	0.87688600
H	-6.83368800	1.25430200	-3.18050000
H	-8.29775400	0.57593200	-1.29835900
C	-1.16353800	-3.26905400	-1.20311100

H	-1.72404700	-3.72635100	-2.02390000
H	-1.29620500	-3.90315200	-0.32000000
H	-1.56886800	-2.28379100	-0.98614400
C	-2.51532400	-0.67244100	-2.63487400
H	-3.46161800	-1.21207800	-2.51535800
O	-2.59809100	1.10825400	0.47613900
H	-2.66059600	0.01185400	-3.48793500
O	0.11851900	0.68514500	-3.20366000
C	0.60693100	-0.18935200	-4.21886100
H	0.49906500	0.27173900	-5.20327900
H	1.66737200	-0.34603700	-4.01608800
H	0.09031700	-1.15468900	-4.19741100
H	-0.80234100	0.91610000	-3.38435200

TS3



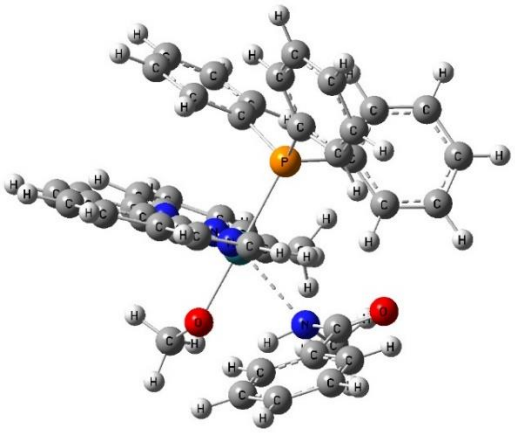
SCF done	-2542.50365101
SCF done for solvent	-2542.55284078
Zero-point correction	0.751185
Thermal correction to Gibbs free energy	0.672309

C	-1.66763200	4.18175800	1.79654500
C	-2.48386000	3.08403800	1.90210700
C	0.39763300	5.19092900	0.80811000
C	-0.49761500	4.08473700	1.01498500
C	1.48570000	5.08445300	0.00214700
C	-2.13557700	1.89009900	1.24150400
C	-0.22831100	2.84951700	0.39896800
C	1.77923100	3.84622500	-0.65778100
C	0.94139900	2.74364100	-0.42686600

C	2.85129400	3.65554700	-1.55757200
C	3.02814400	2.44032400	-2.17669000
C	2.15814100	1.37116300	-1.87226100
C	2.25505600	0.00698900	-2.43596900
C	1.41402100	-2.15741700	-2.43405700
C	3.30251100	-0.35121300	-3.27225600
C	2.44127800	-2.57018500	-3.29461300
C	3.38456200	-1.66201700	-3.73143100
H	-1.91001100	5.11692200	2.29240500
H	-3.39718400	3.11099800	2.48419100
H	0.17023900	6.12985000	1.30326800
H	2.14141700	5.93314200	-0.16354300
H	-2.77040900	1.01835500	1.33332900
H	3.52034600	4.48292000	-1.77331800
H	3.83184000	2.30919700	-2.88952000
H	4.05548200	0.37377400	-3.55283900
H	2.48284200	-3.61235600	-3.59286900
H	4.18734300	-1.96537200	-4.39470700
N	-1.03833000	1.75612800	0.51221600
N	1.17484800	1.54283100	-0.99688700
N	1.29124800	-0.87806400	-2.05052700
Ru	-0.19568200	0.09804300	-0.70328200
H	-1.73301200	-1.94793400	-2.94740800
P	0.98816600	-0.85997400	1.11705000
C	0.70950700	-2.61329700	1.57570000
C	-0.52867000	-3.19775100	1.29840000
C	1.66485700	-3.33203000	2.30464800
C	-0.79221900	-4.50249700	1.71014900
H	-1.29136100	-2.61984400	0.78247700
C	1.40136900	-4.63716900	2.70456600
H	2.61521100	-2.87159600	2.56144000
C	0.17483400	-5.22640400	2.40077800
H	-1.75728300	-4.95013500	1.49556400
H	2.14977200	-5.19163000	3.26106300
H	-0.02983700	-6.24456000	2.71560300
C	0.75930600	-0.05594200	2.75125800
C	-0.56578900	0.03047800	3.19717100
C	1.79516200	0.36306700	3.58911800
C	-0.85004100	0.57008000	4.44626600
H	-1.36946900	-0.35295200	2.57100300
C	1.50367200	0.90737100	4.83881800
H	2.83068100	0.25445200	3.28435600
C	0.18425000	1.02075000	5.26476400
H	-1.87950600	0.62817800	4.78567200
H	2.31392000	1.23200000	5.48350000
H	-0.03665200	1.44231600	6.24000400
C	2.78185000	-0.74971300	0.73610300
C	3.46389400	-1.82613400	0.15469600
C	3.43337100	0.48697700	0.82464700
C	4.76437300	-1.67068200	-0.31699000
H	2.97620500	-2.79323700	0.06855000
C	4.73851100	0.63910700	0.36324200
H	2.91491900	1.34377600	1.25009400
C	5.40649700	-0.43883800	-0.21174400
H	5.27690100	-2.51633700	-0.76466400
H	5.22930100	1.60336000	0.45139100

H	6.42359200	-0.32166400	-0.57138400
N	-2.21809500	-0.99644900	-1.14590700
C	-3.23634600	-0.92624800	-0.17160600
C	-4.63989700	-0.64491900	-0.60911900
C	-5.68662700	-1.02627100	0.23532300
C	-4.91555700	0.04813800	-1.79266700
C	-7.00076300	-0.74012300	-0.11268000
H	-5.45043300	-1.54710300	1.15741100
C	-6.23123400	0.34936800	-2.12823100
H	-4.10167600	0.37426200	-2.43562800
C	-7.27274100	-0.05172500	-1.29399500
H	-7.81379100	-1.04883800	0.53578300
H	-6.44500400	0.89717400	-3.03973300
H	-8.29905800	0.17660800	-1.56284300
C	0.47811300	-3.18468800	-1.87644300
H	-0.00965700	-3.74781800	-2.67704400
H	1.04212700	-3.89795400	-1.26504500
H	-0.27278000	-2.71946200	-1.24395700
C	-2.47389900	-2.04837500	-2.15101700
H	-2.38038900	-3.04912400	-1.71611700
O	-2.98219100	-1.03939000	1.01750200
H	-3.47068900	-1.96191800	-2.59512100
O	-1.39539700	0.99344400	-2.25534900
C	-0.95942800	0.94743400	-3.58723400
H	-1.73989700	1.32333700	-4.26055800
H	-0.07235500	1.58411300	-3.72776900
H	-0.68706800	-0.06969000	-3.91392700
H	-2.09806000	0.00566000	-1.80269300

I7

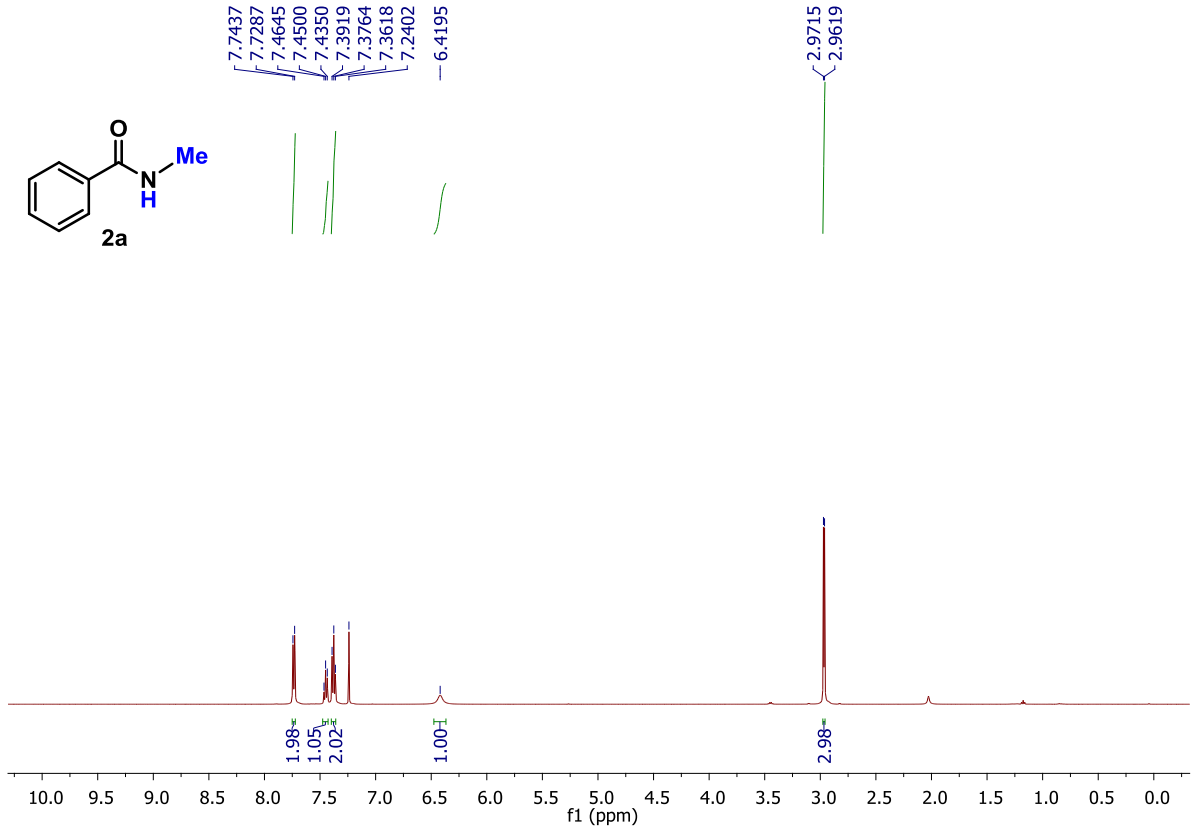


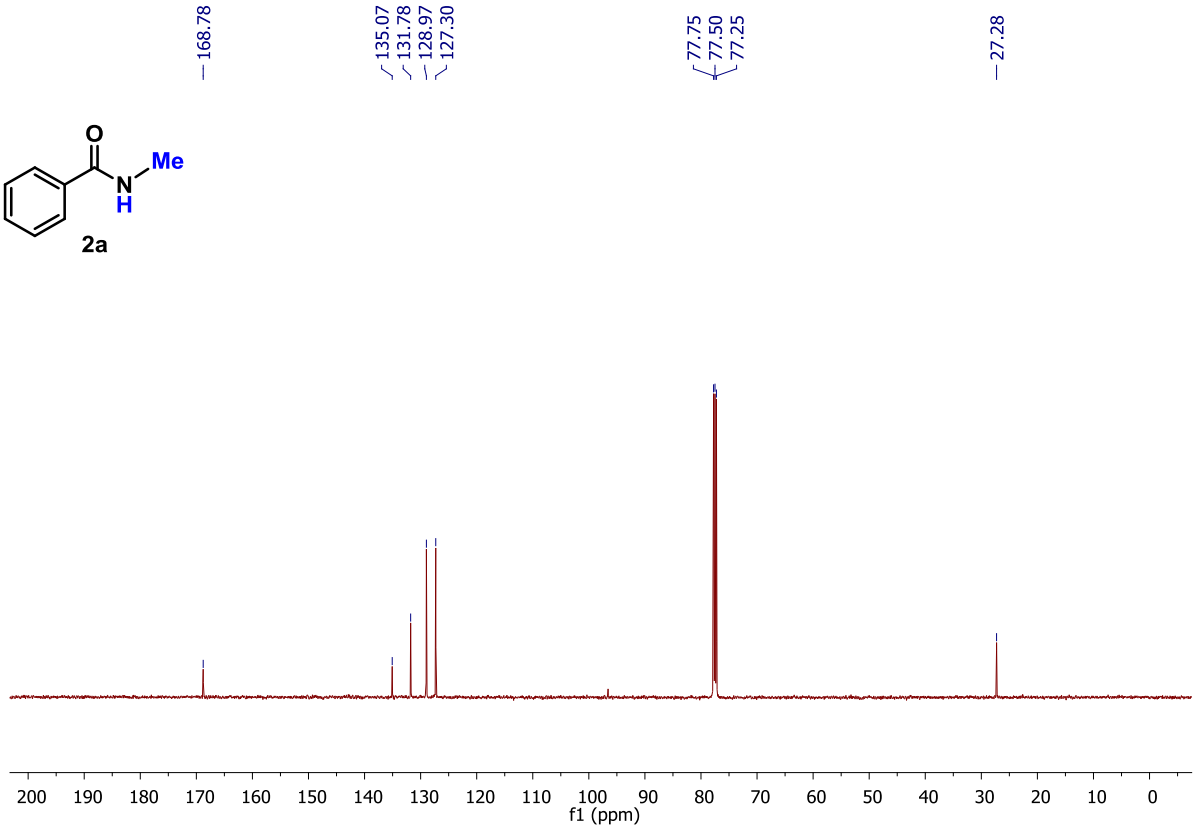
SCF done	-2542.51315955
SCF done for solvent	-2542.56331852
Zero-point correction	0.756169
Thermal correction to Gibbs free energy	0.676745

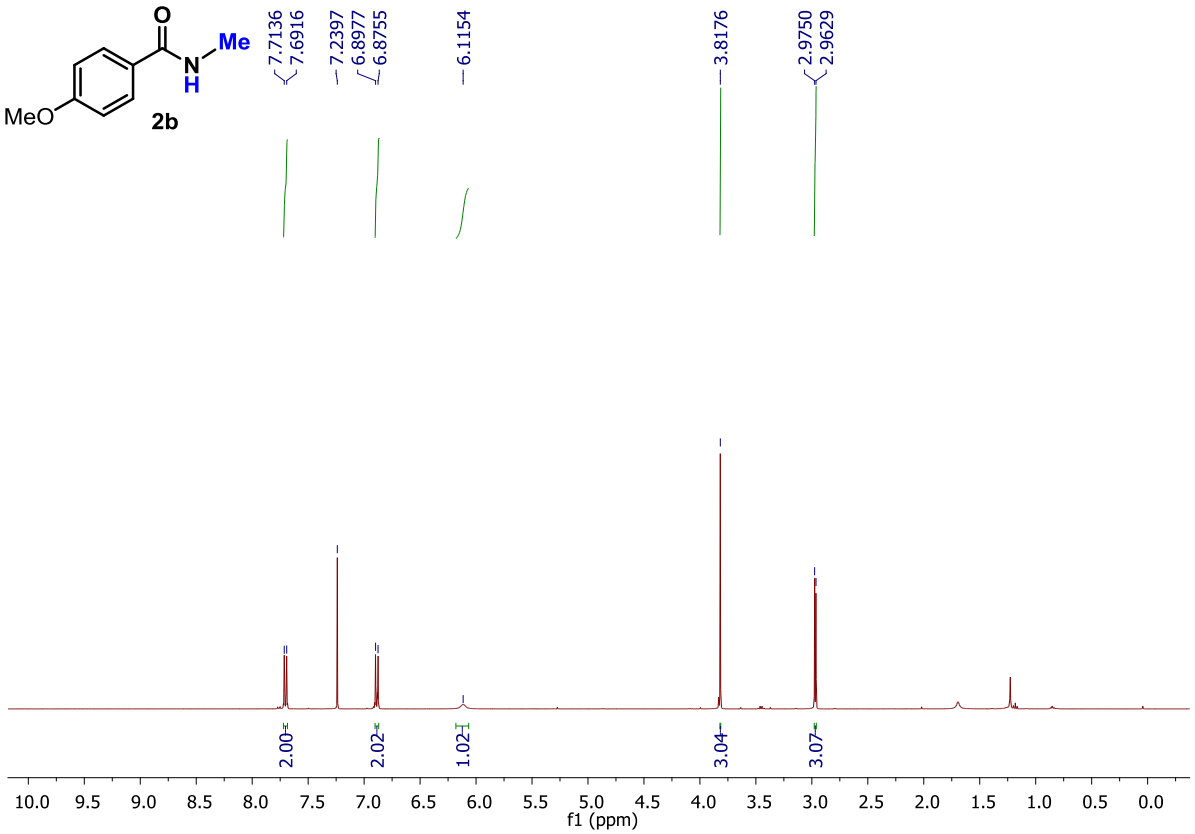
C	3.67046600	-1.96377100	2.06463700
C	3.73659600	-0.62453100	1.76579300
C	2.37014700	-4.10584700	1.90901500
C	2.56335800	-2.71232300	1.61063600
C	1.26745200	-4.77711200	1.48413100
C	2.72828500	-0.04389400	0.97423100
C	1.60325900	-2.03912000	0.83776500
C	0.24855700	-4.10369800	0.73093500
C	0.42681600	-2.74612500	0.42656700
C	-0.93541300	-4.71117700	0.25706700
C	-1.84545300	-3.97814300	-0.46891700
C	-1.60268100	-2.60906600	-0.71472100
C	-2.49047800	-1.71259800	-1.48570900
C	-2.79886400	0.38913700	-2.41125300
C	-3.76612200	-2.11411600	-1.85400300
C	-4.08593600	0.02957700	-2.83673000
C	-4.57462000	-1.23157900	-2.56331200
H	4.44311100	-2.44760100	2.65462000
H	4.55552400	-0.00250900	2.10673500
H	3.13312500	-4.61495800	2.48960700
H	1.13590000	-5.82952000	1.71378000
H	2.77383700	1.00863100	0.73029200
H	-1.11310400	-5.76372500	0.45509600
H	-2.73441600	-4.45386600	-0.86283900
H	-4.13587100	-3.09299400	-1.57713000
H	-4.68562900	0.76457900	-3.36293300
H	-5.57234300	-1.52383300	-2.87245000
N	1.70819600	-0.72712800	0.48273400
N	-0.50357000	-2.03401400	-0.24525400
N	-1.99642300	-0.47732000	-1.77795800
Ru	0.05640900	-0.20373600	-0.84095100
H	0.08906700	1.62242700	-3.88980800
P	-1.07328900	0.98972500	0.93052600
C	-1.51812500	2.74701400	0.65980800
C	-0.69827600	3.49579800	-0.18802100
C	-2.53295700	3.38936900	1.37926300
C	-0.91117200	4.86271700	-0.34910000
H	0.13188100	3.01986200	-0.70411100
C	-2.75539700	4.75121900	1.20333900
H	-3.14413200	2.82829600	2.08113300
C	-1.95001200	5.48747100	0.33453600
H	-0.25659600	5.43337500	-1.00030100
H	-3.55011900	5.24273300	1.75480800
H	-2.12389200	6.55088900	0.20641300
C	-0.21778200	1.15715100	2.55362600
C	0.94651500	1.93789500	2.54593400
C	-0.66641400	0.62136100	3.76172400
C	1.66849100	2.14337900	3.71503500
H	1.27125000	2.41501300	1.62198200
C	0.06156600	0.82747500	4.93340200
H	-1.59430700	0.06303100	3.80867500
C	1.23236100	1.57679600	4.91193100
H	2.56301100	2.75774600	3.69574500
H	-0.30014800	0.40967900	5.86728100
H	1.79217700	1.73866100	5.82714100

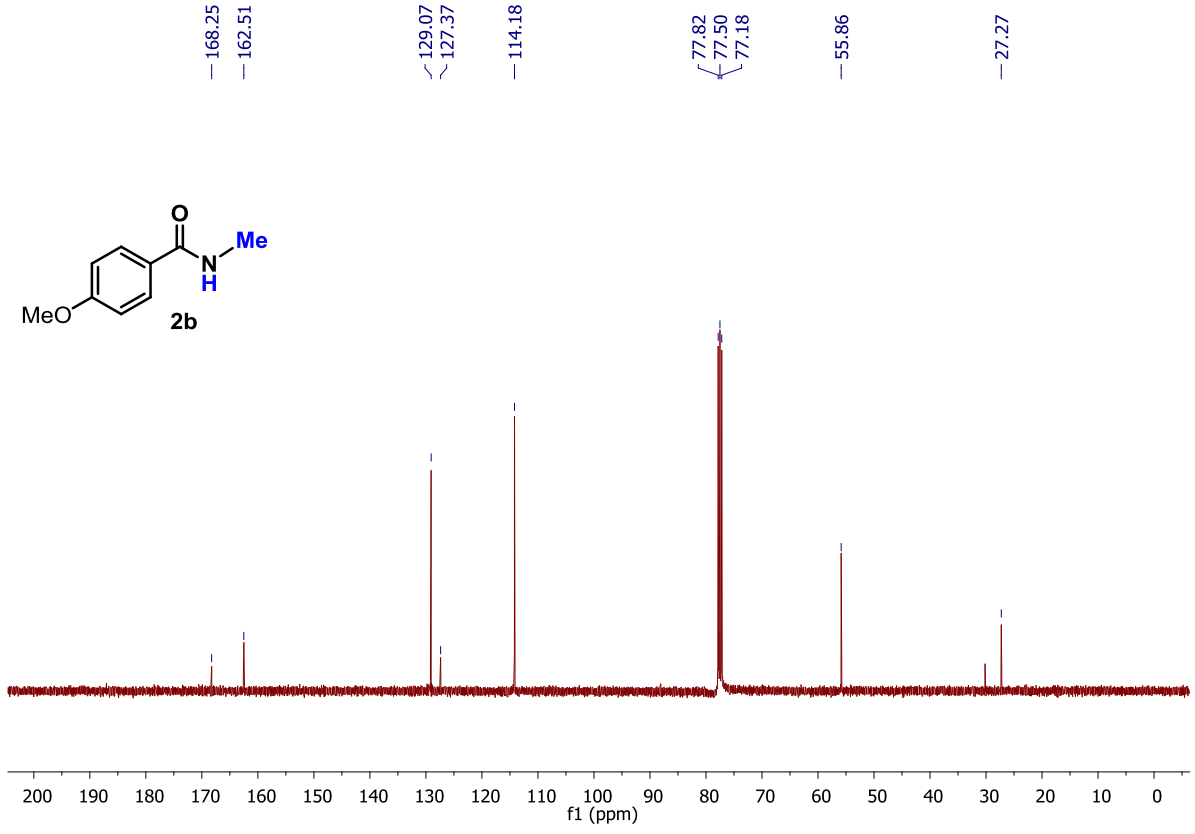
C	-2.64623100	0.10659100	1.26218500
C	-3.86272300	0.54868500	0.72885000
C	-2.60378300	-1.15071900	1.88058100
C	-5.00943500	-0.23404000	0.83576000
H	-3.91712200	1.50773600	0.22199900
C	-3.75343300	-1.92657600	1.99932800
H	-1.66069800	-1.53485300	2.26347500
C	-4.96086900	-1.46908300	1.47716900
H	-5.94399700	0.12663100	0.41765800
H	-3.70114400	-2.89091000	2.49495500
H	-5.85876400	-2.07168200	1.56846000
N	1.39032700	1.34737200	-2.27645800
C	2.49792300	1.95863700	-1.64777500
C	3.77916200	1.19023700	-1.52850200
C	4.86271600	1.87850900	-0.96835500
C	3.92247600	-0.14825500	-1.91108000
C	6.07881700	1.23440000	-0.78389100
H	4.72579400	2.91672300	-0.68447500
C	5.14639900	-0.78612700	-1.72197400
H	3.08293500	-0.71910000	-2.30411200
C	6.22071300	-0.10178100	-1.16000000
H	6.91811200	1.77233100	-0.35538500
H	5.25711300	-1.82484800	-2.01550000
H	7.17222000	-0.60497200	-1.01980300
C	-2.32736500	1.79271100	-2.62673900
H	-2.25778800	2.02350500	-3.69406700
H	-3.03398800	2.49953800	-2.17958800
H	-1.35956200	1.94333700	-2.15769600
C	0.81080000	2.21090400	-3.32392200
H	0.31649000	3.07842300	-2.88587200
O	2.40272200	3.10111200	-1.23948600
H	1.59098400	2.56681500	-4.00416800
O	1.05218900	-1.27085900	-2.34815000
C	0.31683200	-1.81939100	-3.39431000
H	0.99320000	-2.27046100	-4.13390800
H	-0.36786800	-2.62409000	-3.06796000
H	-0.30427000	-1.07441100	-3.92747600
H	1.58136800	0.40070700	-2.64629300

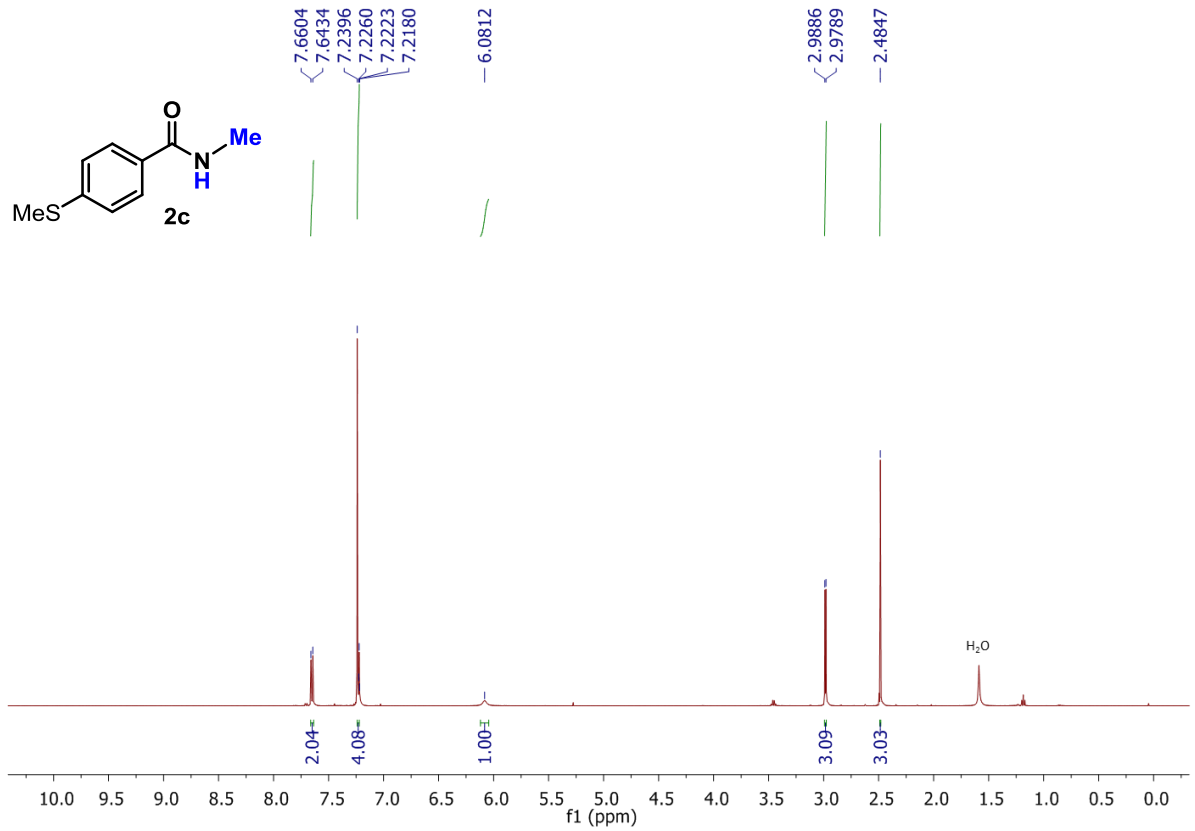
13. Copies of ^{1}H and ^{13}C NMR of the N-Methylated Amides

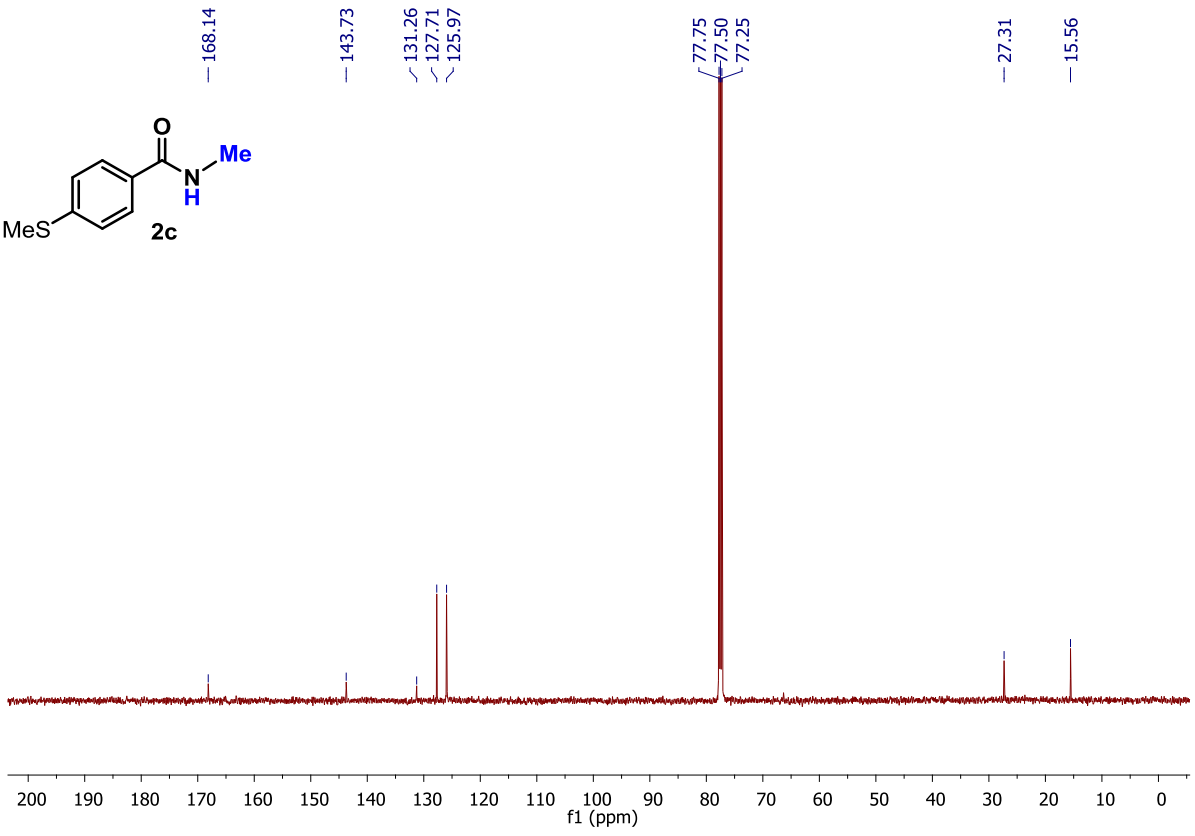


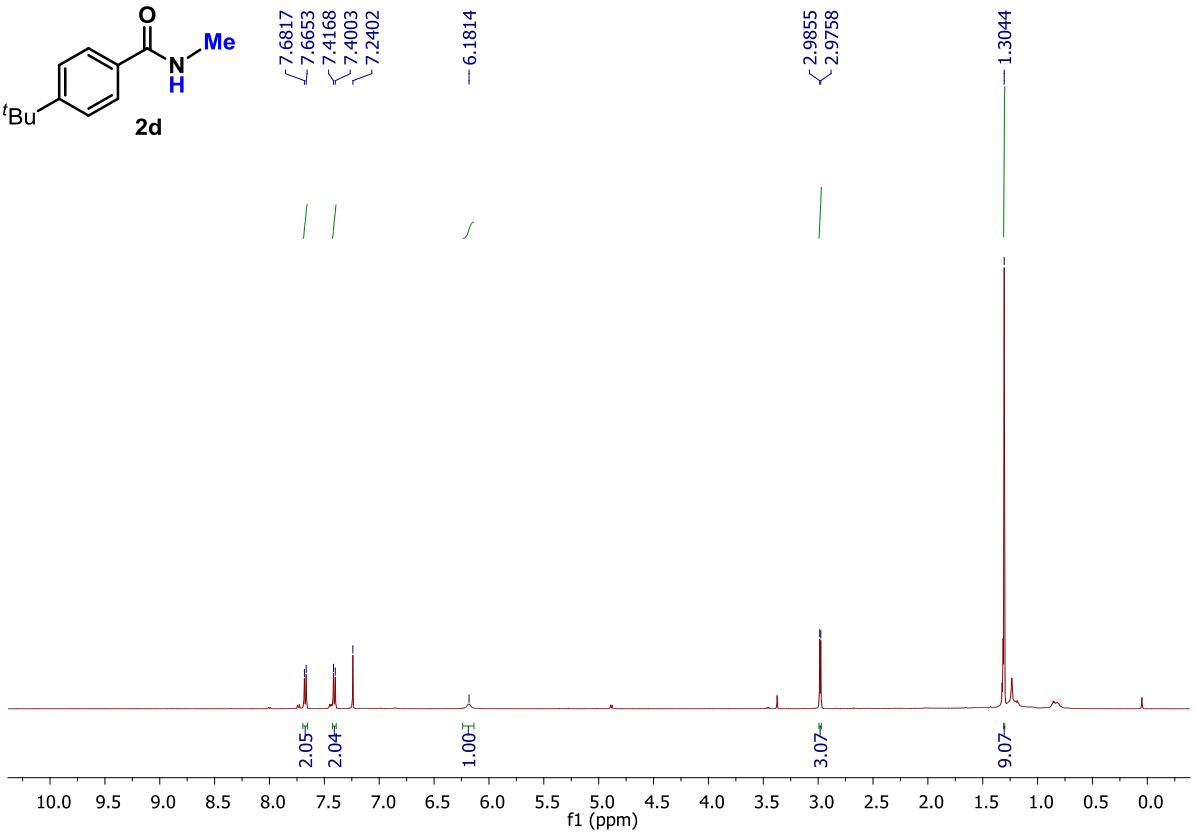


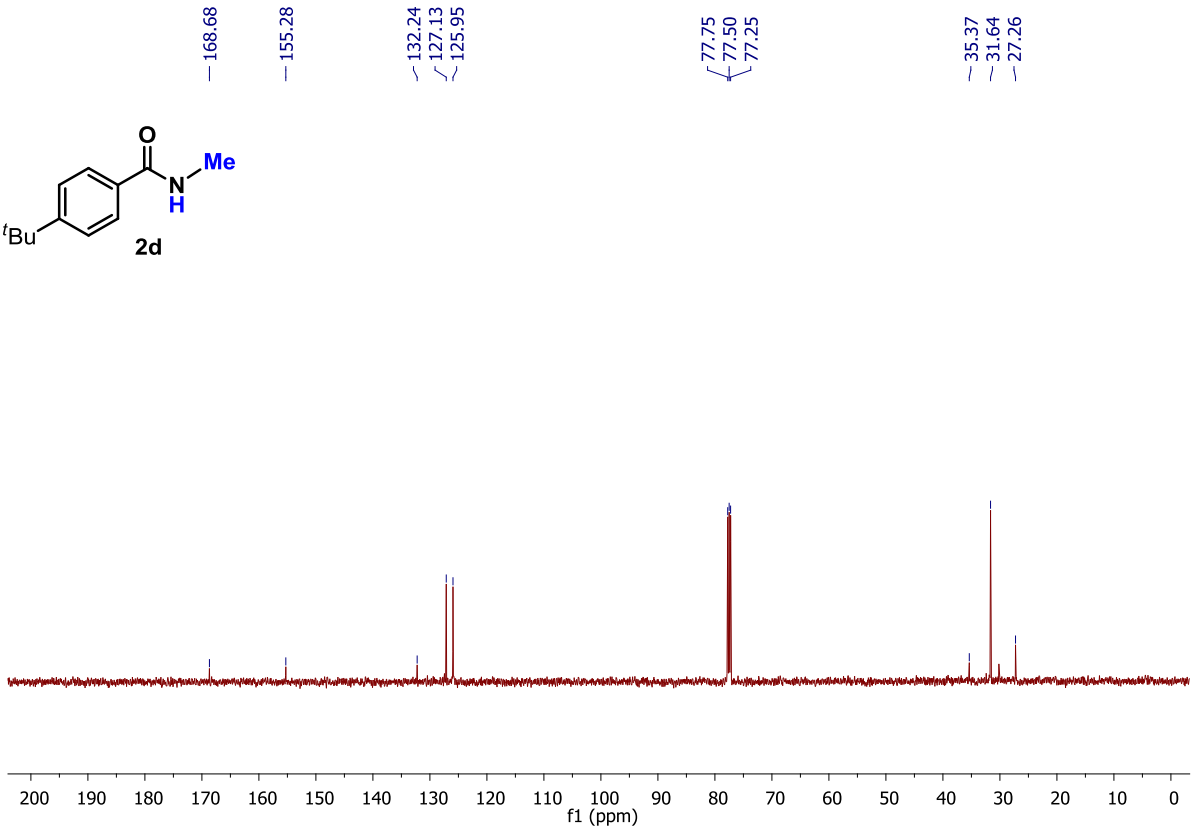

O
N
H
Me
MeO
2b
7.7136
7.6916
7.2397
6.8977
6.8755
6.1154
3.8176
2.9750
2.9629
2.00
2.02
1.02
3.04
3.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

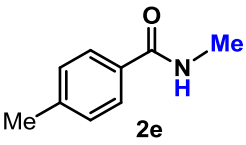

168.25
162.51
129.07
127.37
114.18
77.82
77.50
77.18
55.86
27.27
O
N
H
Me
MeO
2b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.6604
7.6434
7.2396
7.2260
7.2223
7.2180
6.0812
2.9886
2.9789
2.4847
O
N
H
Me
MeS
2c
H2O
2.04
4.08
1.00
3.09
3.03
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
f1 (ppm)

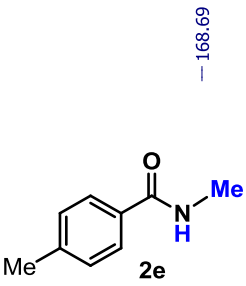

168.14
143.73
131.26
127.71
125.97
77.75
77.50
77.25
27.31
15.56
O
N
H
Me
MeS
2c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N
H
Me
tBu
2d
7.6817
7.6653
7.4168
7.4003
7.2402
6.1814
2.9855
2.9758
1.3044
2.05
2.04
1.00
3.07
9.07
f1 (ppm)

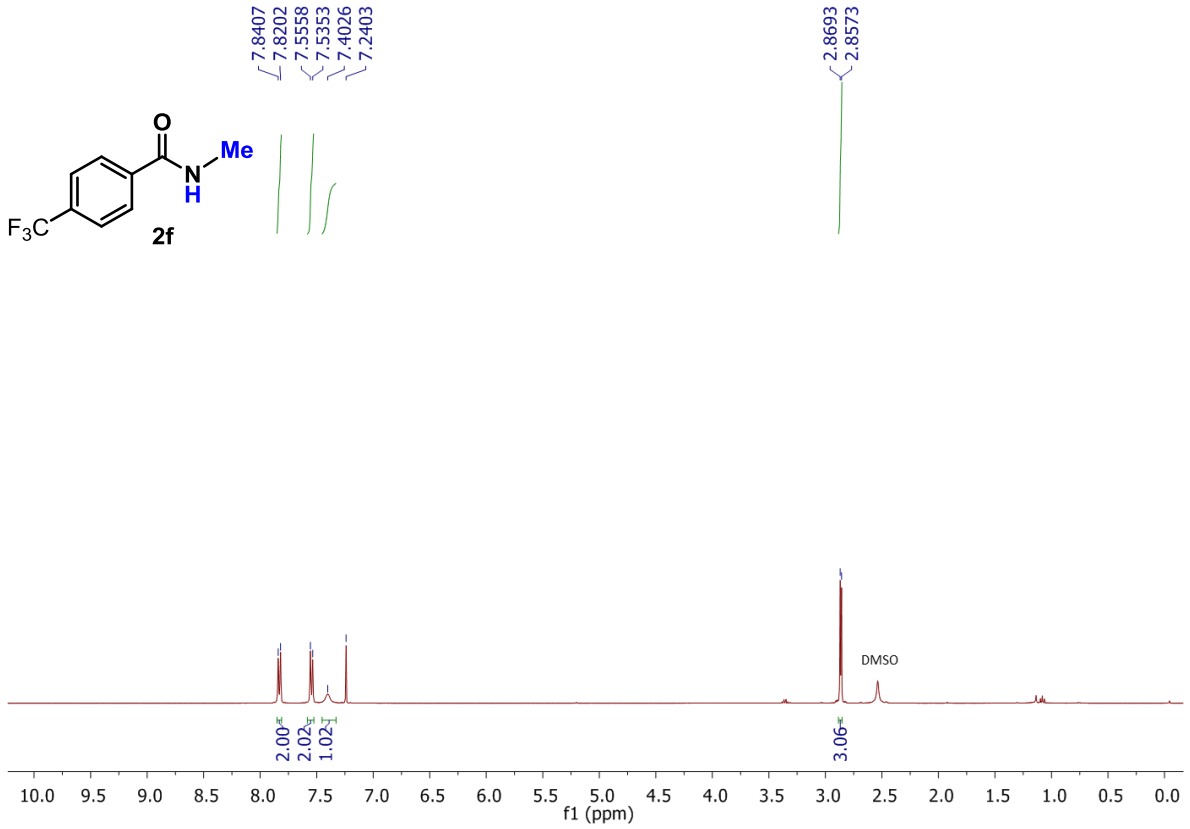

168.68
155.28
132.24
127.13
125.95
77.75
77.50
77.25
35.37
31.64
27.26
O
N
H
Me
tBu
2d
f1 (ppm)

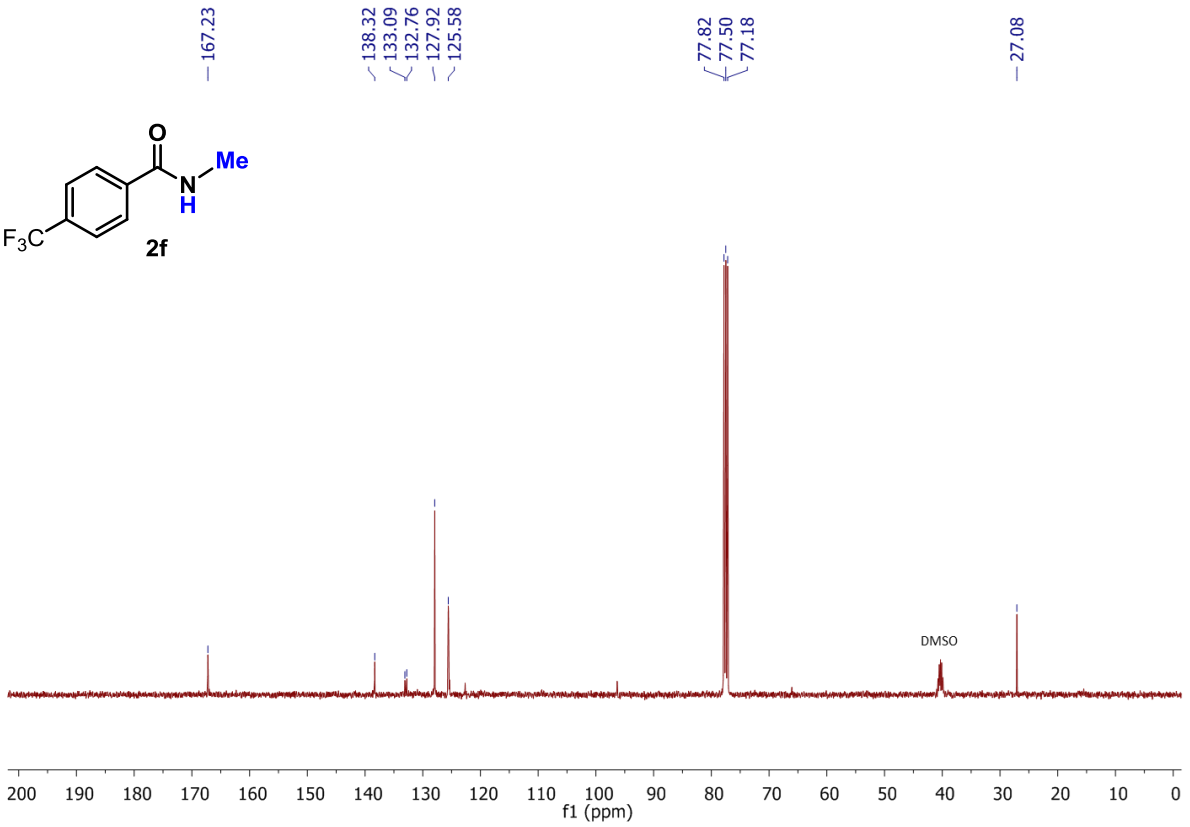

O
Me
N
H
Me
2e

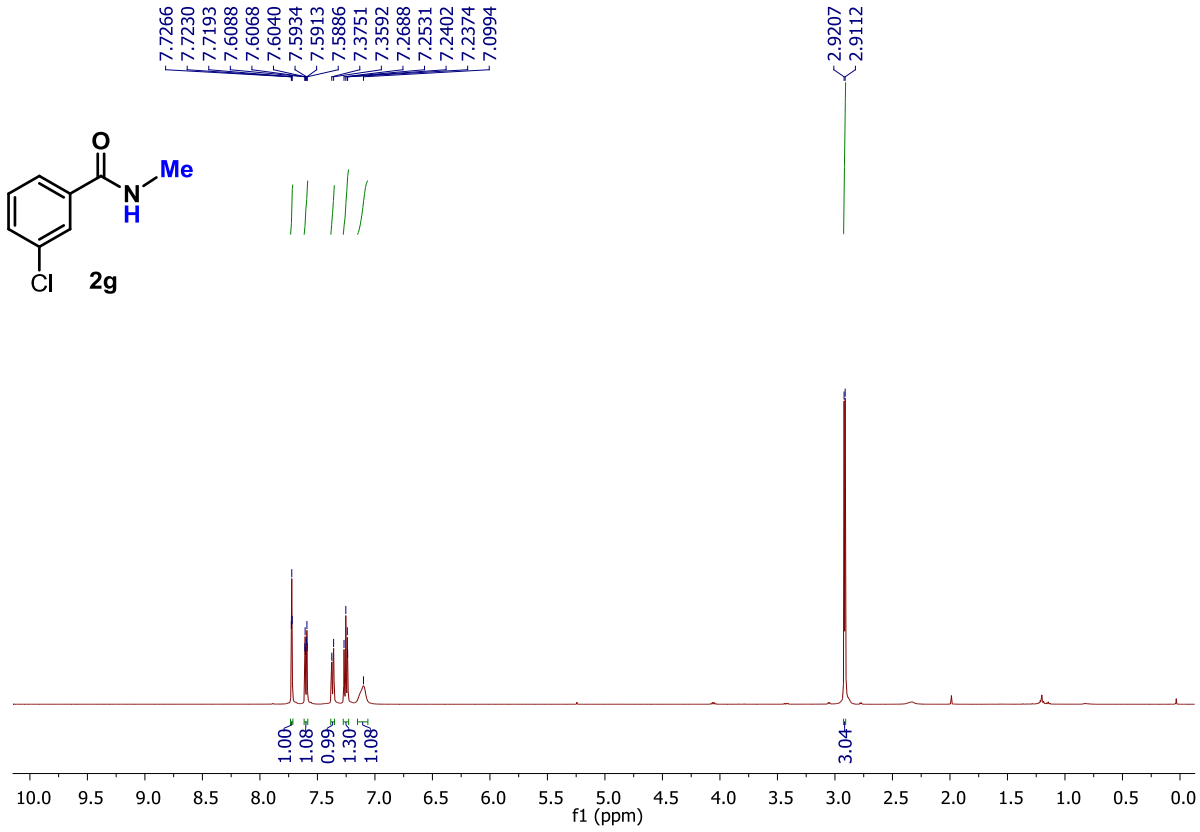
7.6491
7.6285
7.2401
7.1605
7.1405
6.5495
2.9360
2.9240
2.3287
2.00
2.05
1.09
3.04
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

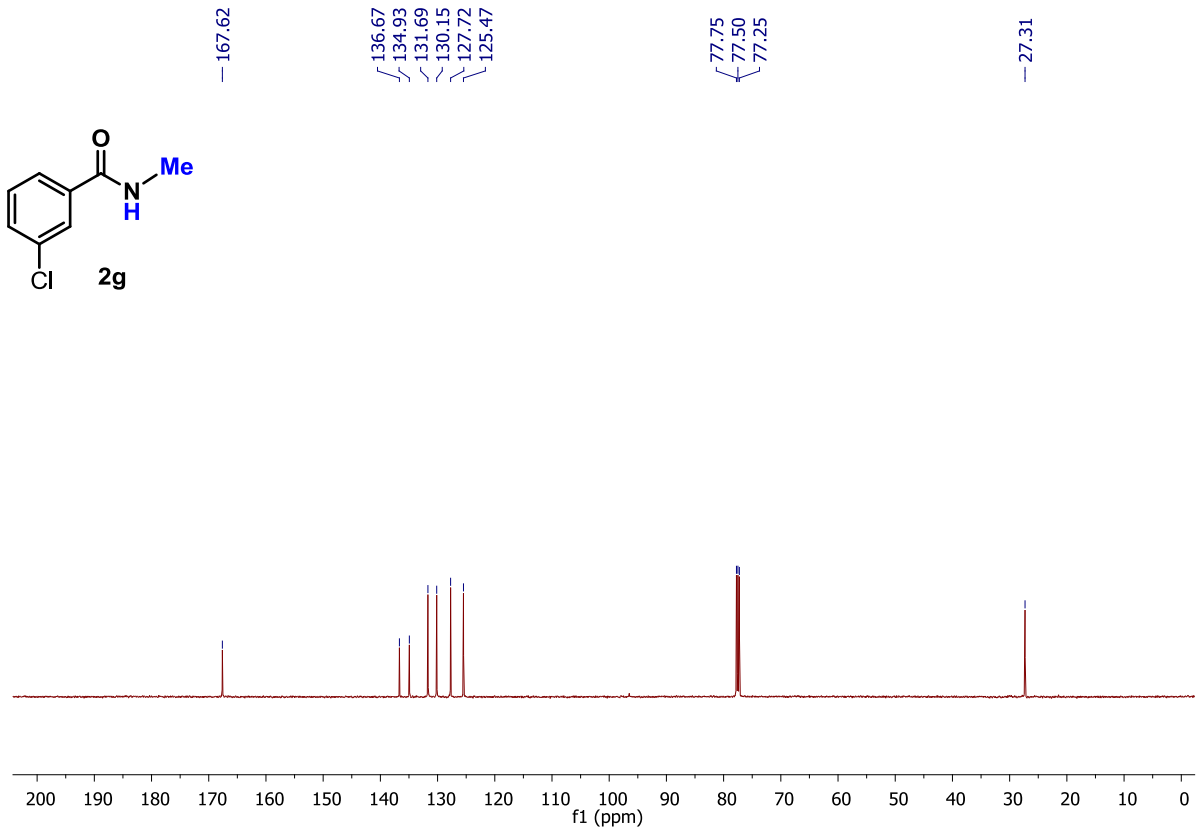

O
Me
N
H
Me
2e

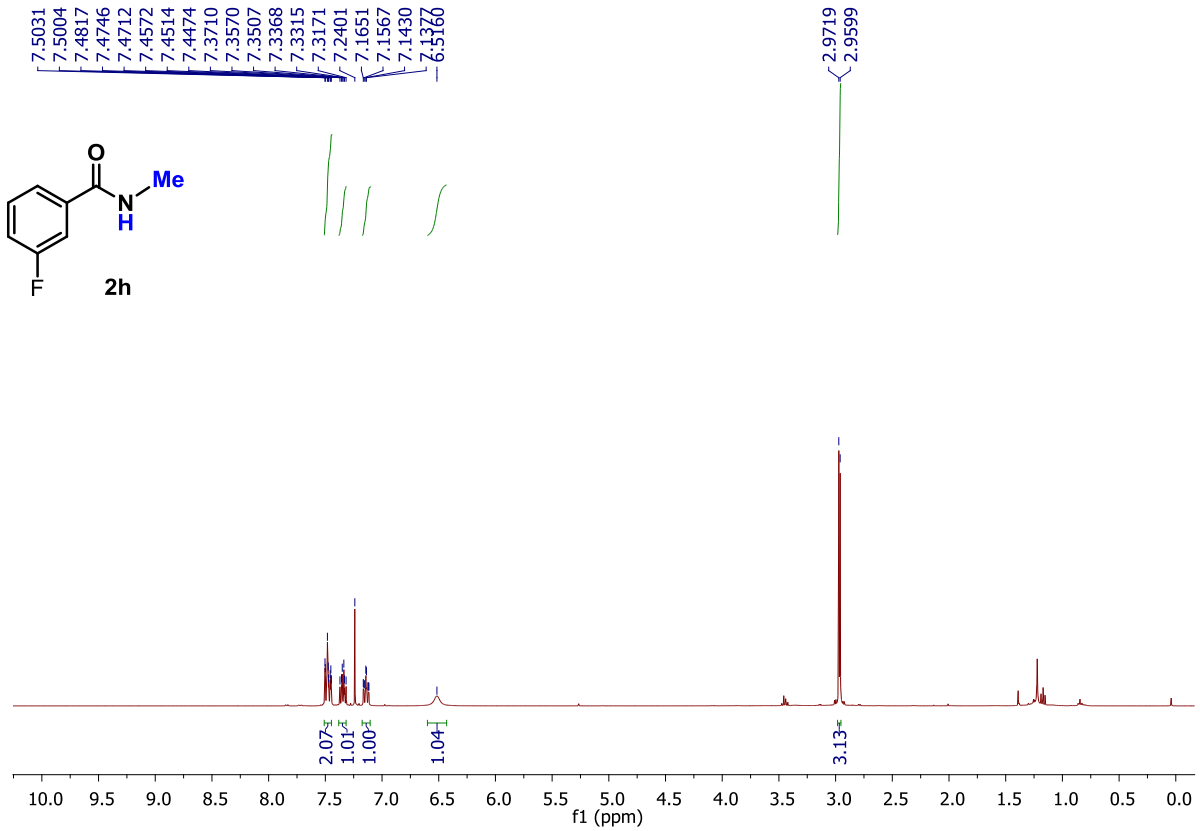
168.69
142.01
132.14
129.53
127.31
77.82
77.50
77.18
27.17
21.80
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

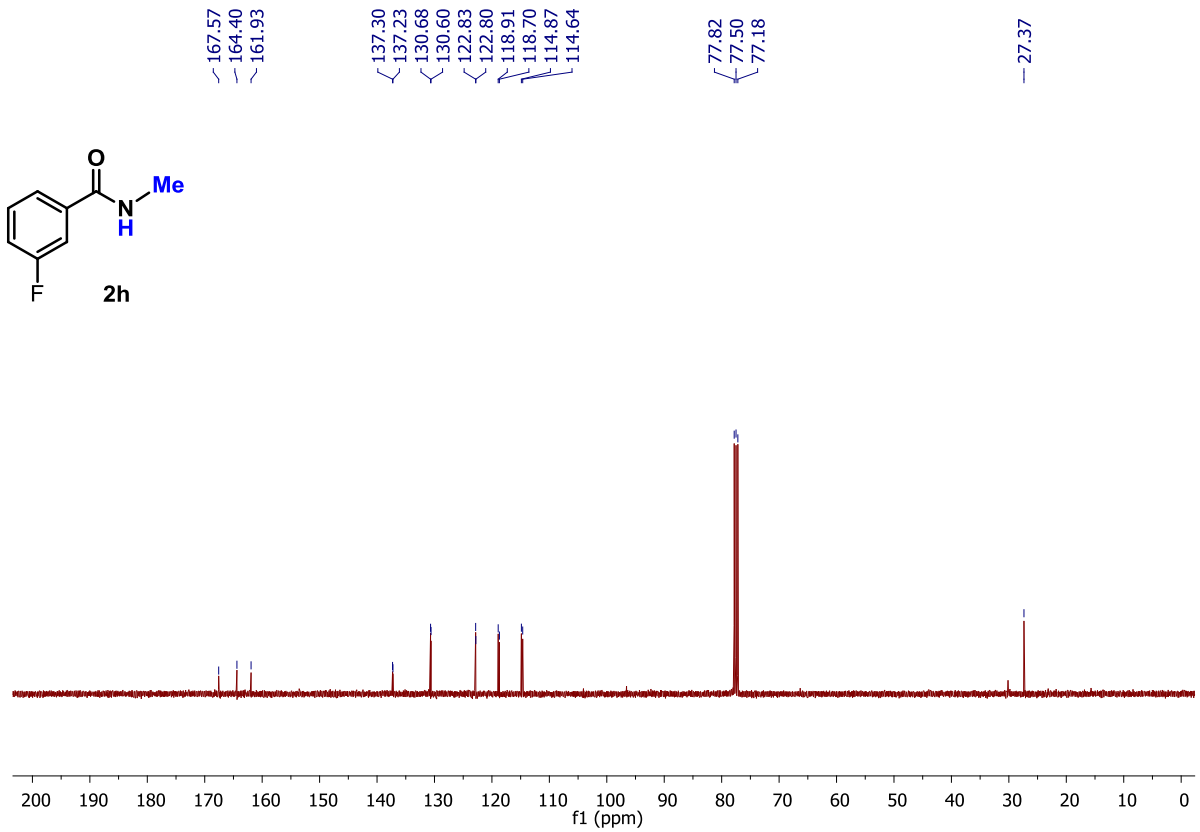

7.8407
7.8202
7.5558
7.5353
7.4026
7.2403
2.8693
2.8573
O
Me
N
H
F3C
2f
DMSO
2.00
2.02
1.02
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

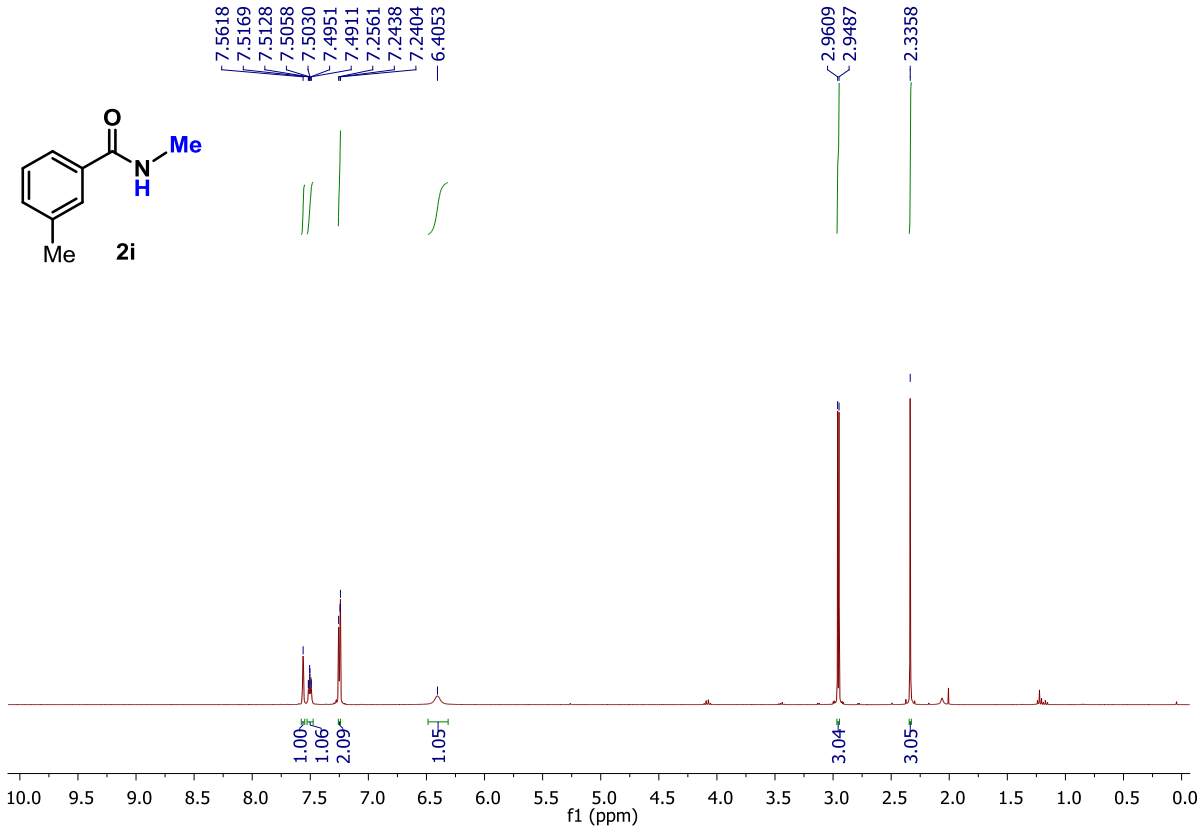

167.23
138.32
133.09
132.76
127.92
125.58
77.82
77.50
77.18
27.08
O
Me
N
H
F3C
2f
DMSO
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

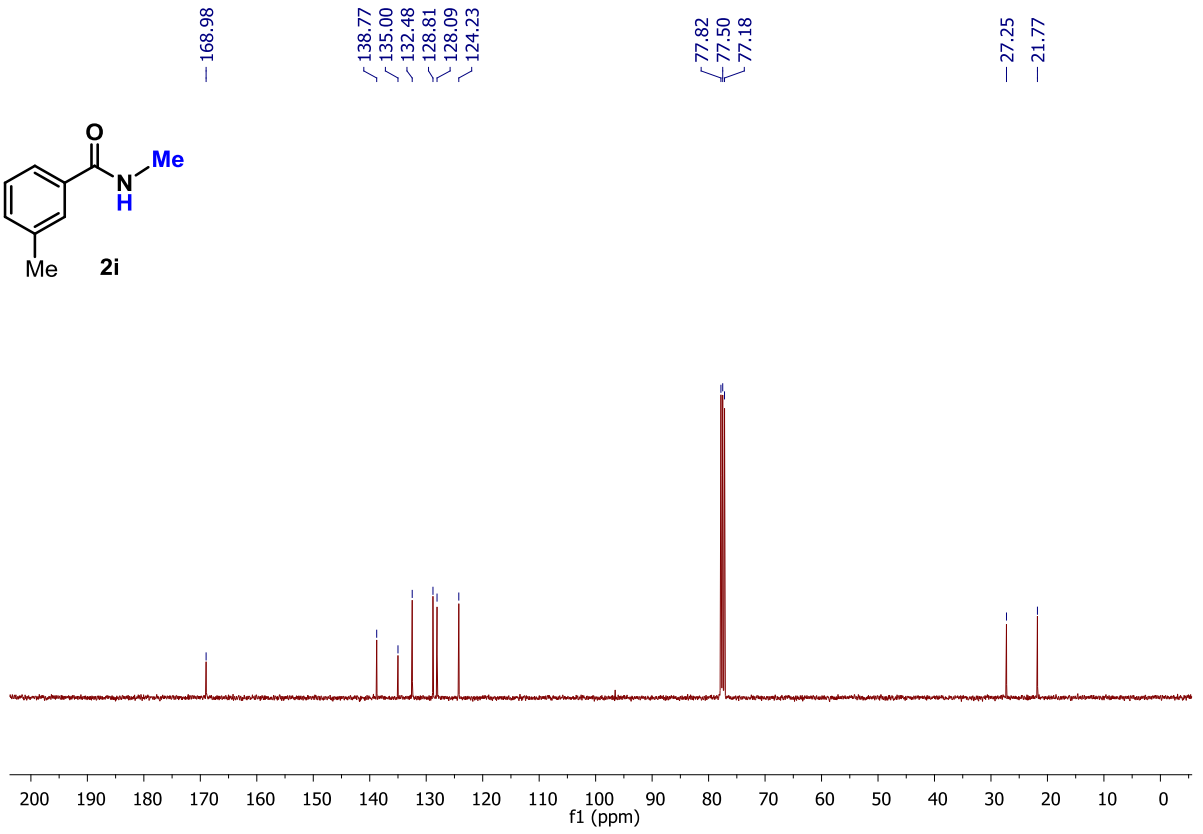

7.7266
7.7230
7.7193
7.6088
7.6068
7.6040
7.5934
7.5913
7.5886
7.3751
7.3592
7.2688
7.2531
7.2402
7.2374
7.0994
2.9207
2.9112
O
N
H
Me
Cl
2g
1.00
1.08
0.99
1.30
1.08
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


167.62
136.67
134.93
131.69
130.15
127.72
125.47
77.75
77.50
77.25
27.31
O
N
H
Me
Cl
2g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.5031
7.5004
7.4817
7.4746
7.4712
7.4572
7.4514
7.4474
7.3710
7.3570
7.3507
7.3368
7.3315
7.3171
7.2401
7.1651
7.1567
7.1430
7.1377
6.5160
2.9719
2.9599
O
Me
N
H
F
2h
2.07
1.01
1.00
1.04
3.13
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
f1 (ppm)


167.57
164.40
161.93
137.30
137.23
130.68
130.60
122.83
122.80
118.91
118.70
114.87
114.64
77.82
77.50
77.18
27.37
O
Me
N
H
F
2h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.5618
7.5169
7.5128
7.5058
7.5030
7.4951
7.4911
7.2561
7.2438
7.2404
6.4053
2.9609
2.9487
2.3358
O
N
H
Me
Me
2i
1.00
1.06
2.09
1.05
3.04
3.05
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
f1 (ppm)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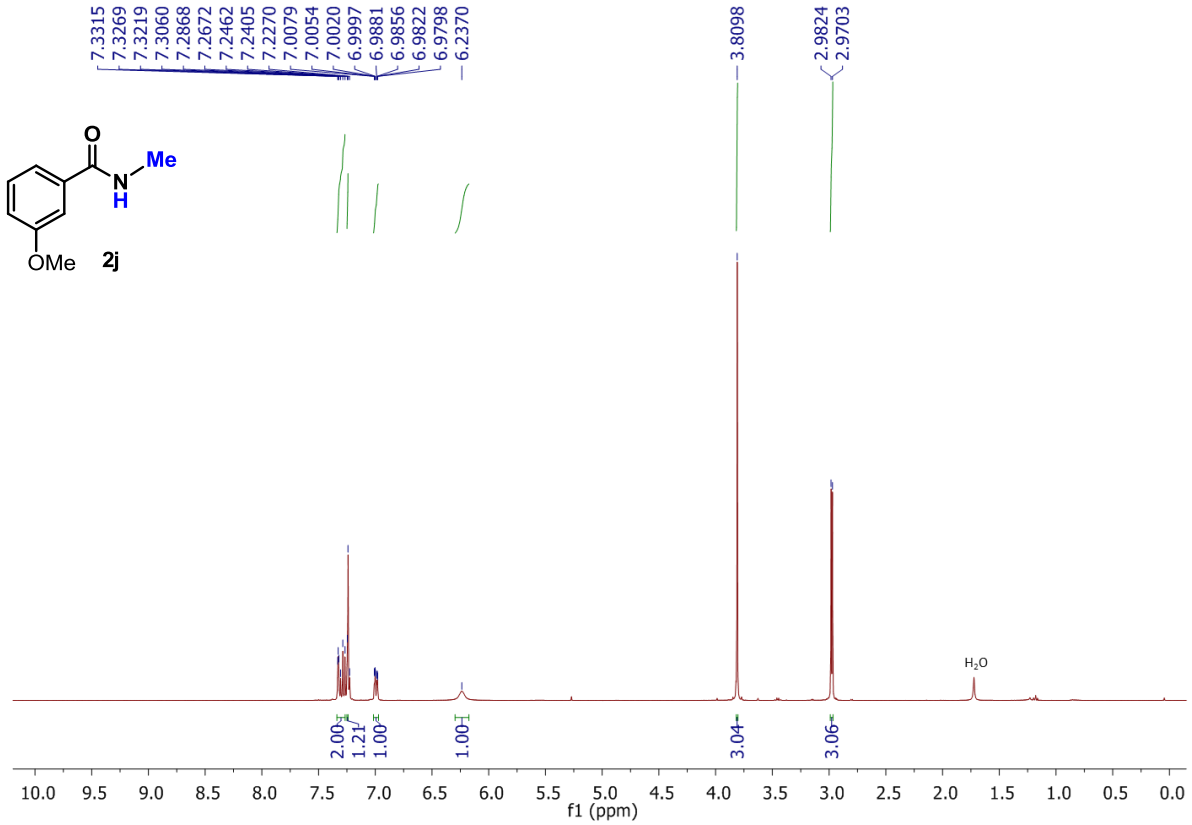
135.00
132.48
128.81
128.09
124.23
77.82
77.50
77.18
27.25
21.77
O
N
H
Me
Me
2i
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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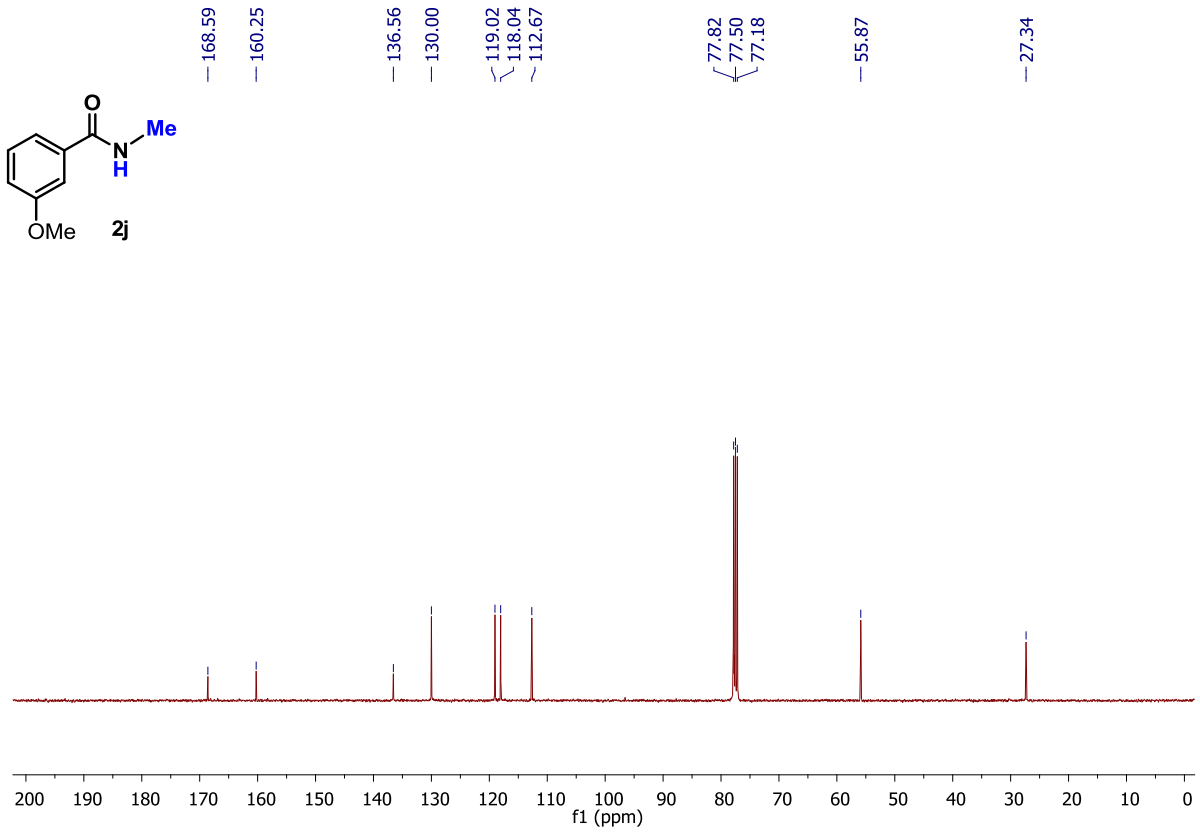
7.3269
7.3219
7.3060
7.2868
7.2672
7.2462
7.2405
7.2270
7.0079
7.0054
7.0020
6.9997
6.9881
6.9856
6.9822
6.9798
6.2370
3.8098
2.9824
2.9703
O
N
H
Me
OMe
2j
H2O
2.00
1.21
1.00
1.00
3.04
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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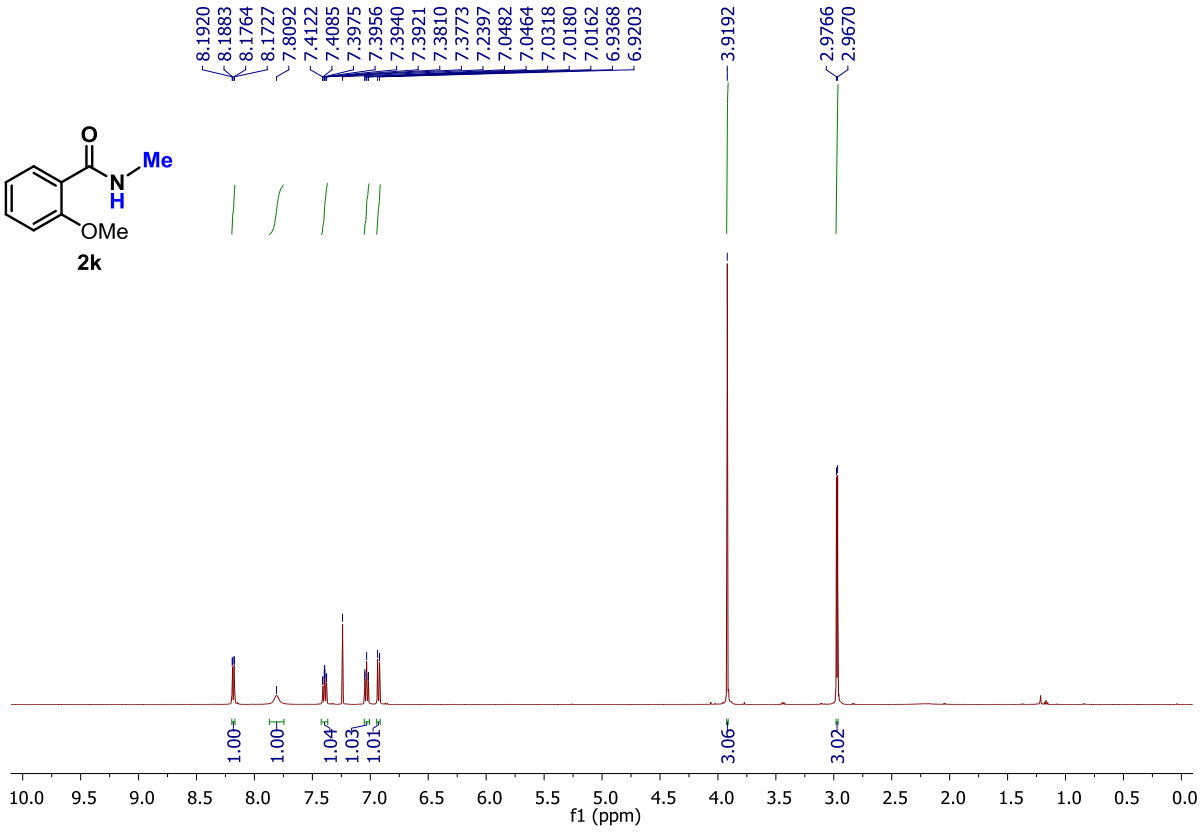
160.25
136.56
130.00
119.02
118.04
112.67
77.82
77.50
77.18
55.87
27.34
O
N
H
Me
OMe
2j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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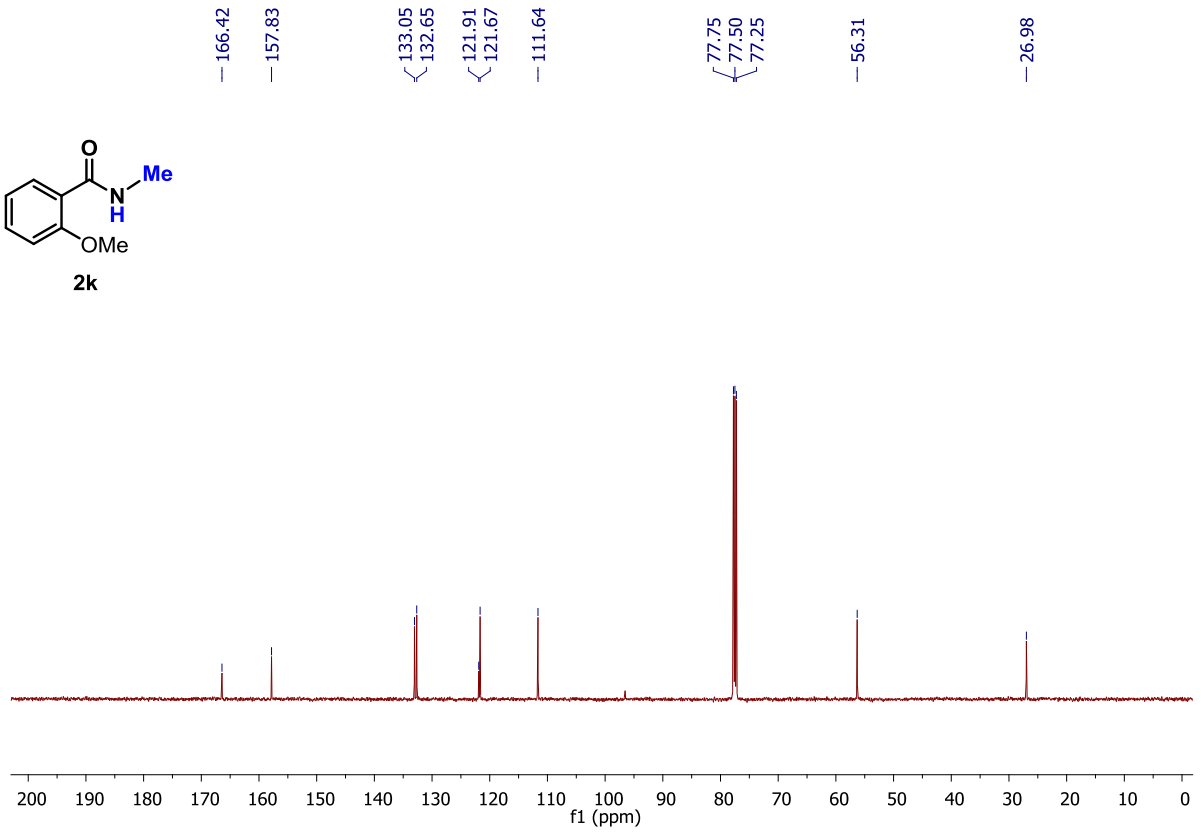
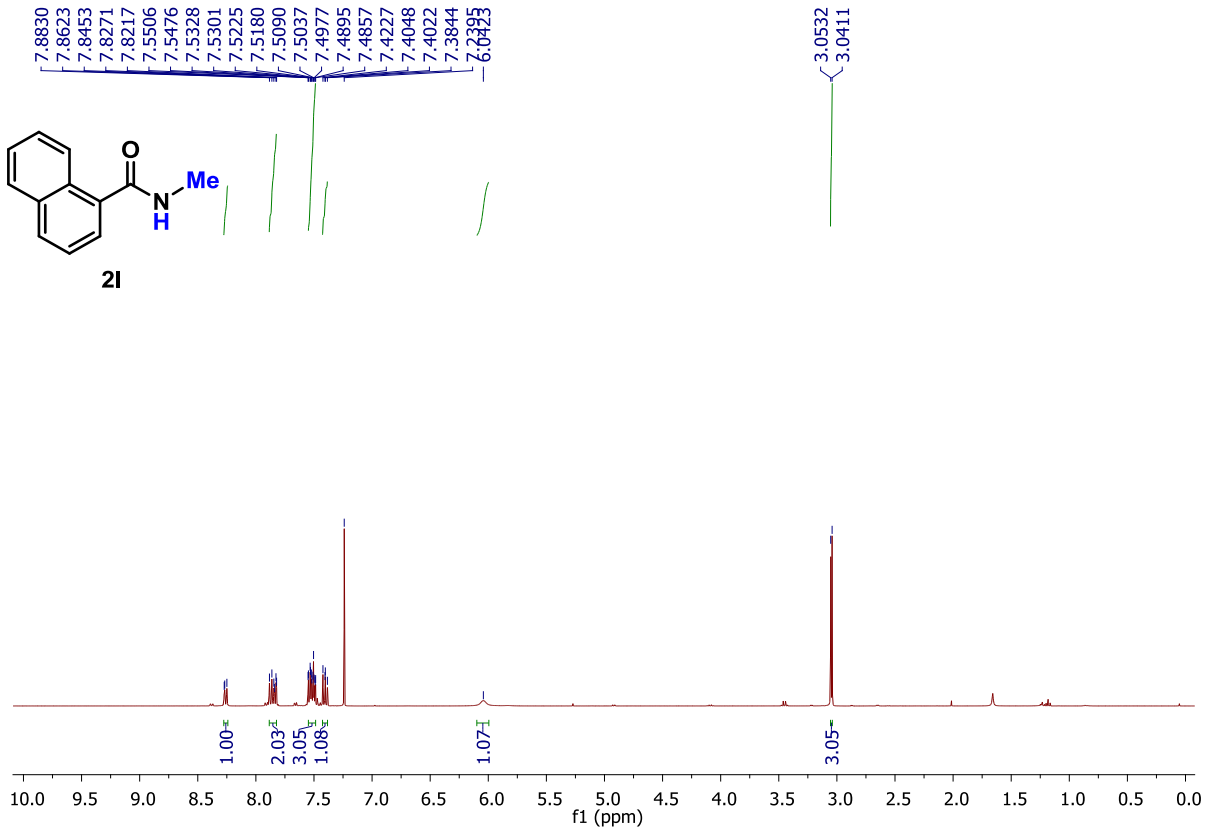
8.1883
8.1764
8.1727
7.8092
7.4122
7.4085
7.3975
7.3956
7.3940
7.3921
7.3810
7.3773
7.2397
7.0482
7.0464
7.0318
7.0180
7.0162
6.9368
6.9203
3.9192
2.9766
2.9670
O
Me
N
H
OMe
2k
1.00
1.00
1.04
1.03
1.01
3.06
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.42
157.83
133.05
132.65
121.91
121.67
111.64
77.75
77.50
77.25
56.31
26.98
O
Me
N
H
OMe
2k
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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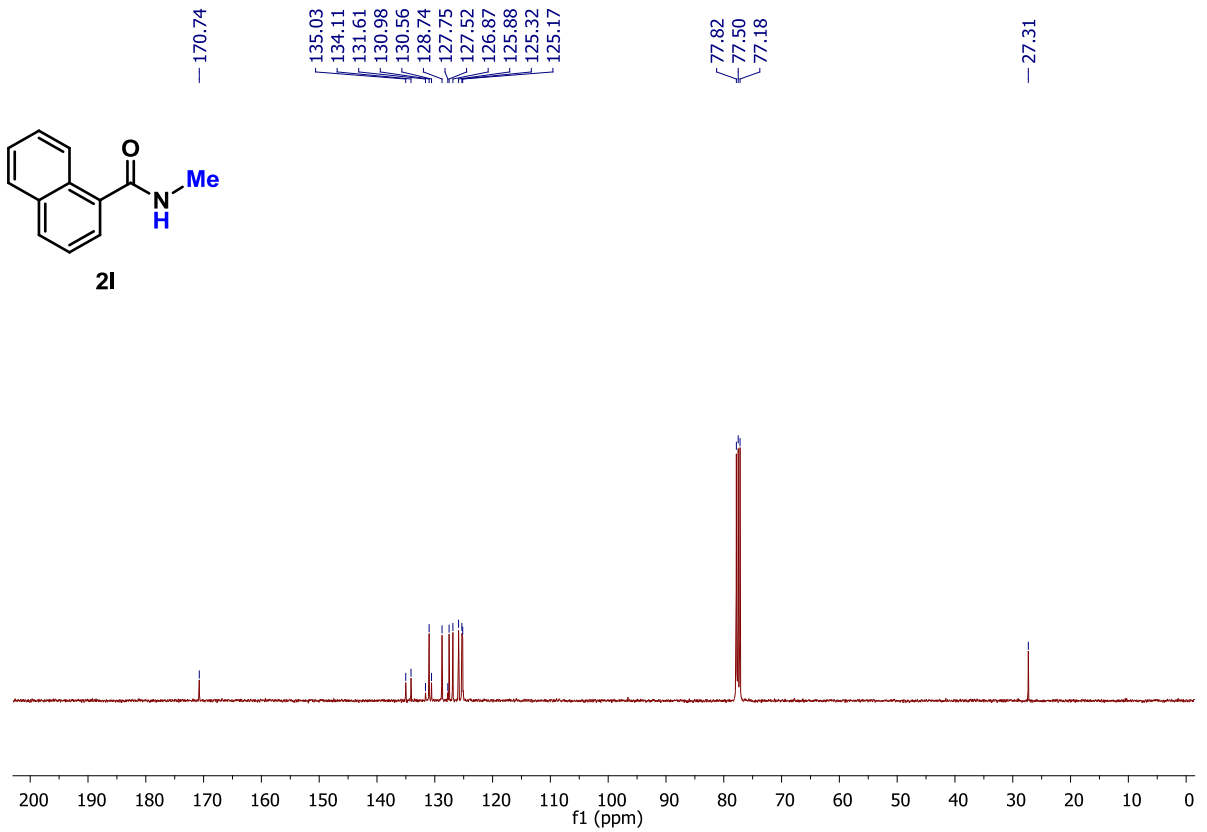
7.8453
7.8271
7.8217
7.5506
7.5476
7.5328
7.5301
7.5225
7.5180
7.5090
7.5037
7.4977
7.4895
7.4857
7.4227
7.4048
7.4022
7.3844
7.2395
6.0423
3.0532
3.0411
O
N
H
Me
2l
1.00
2.03
3.05
1.08
1.07
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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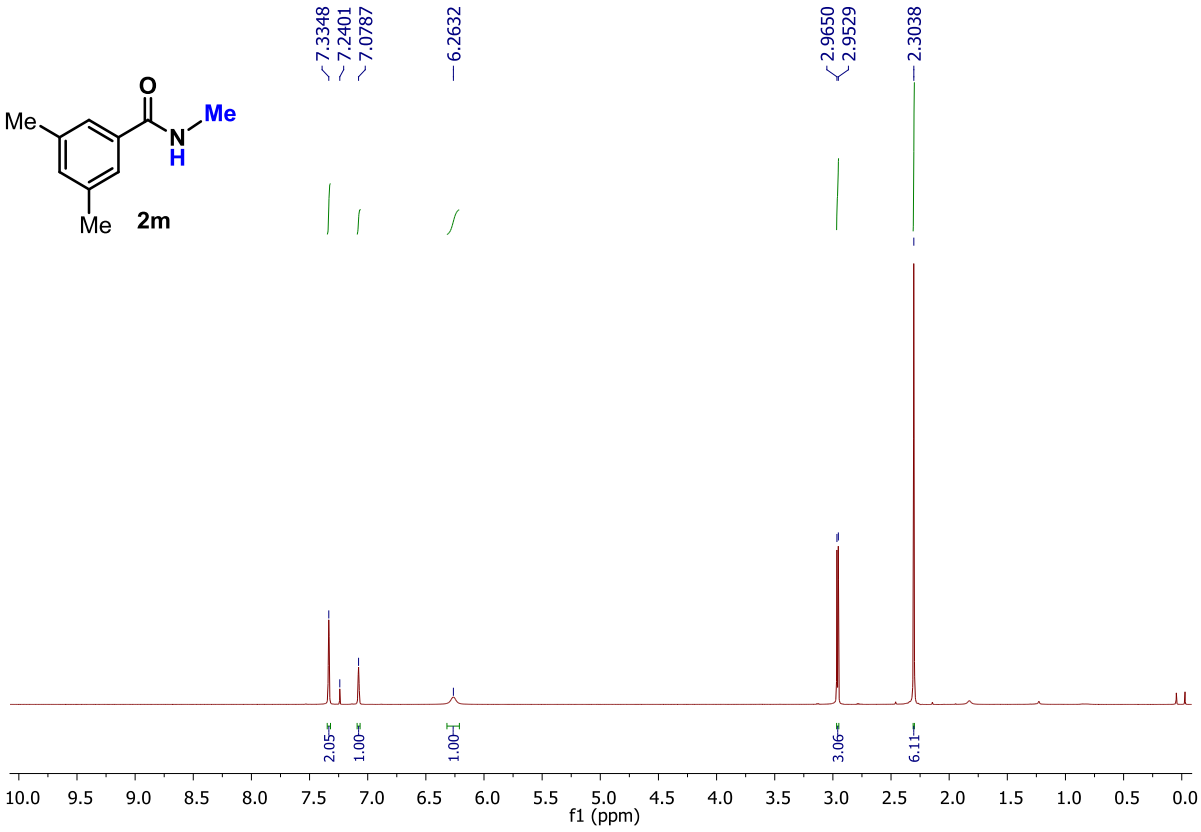
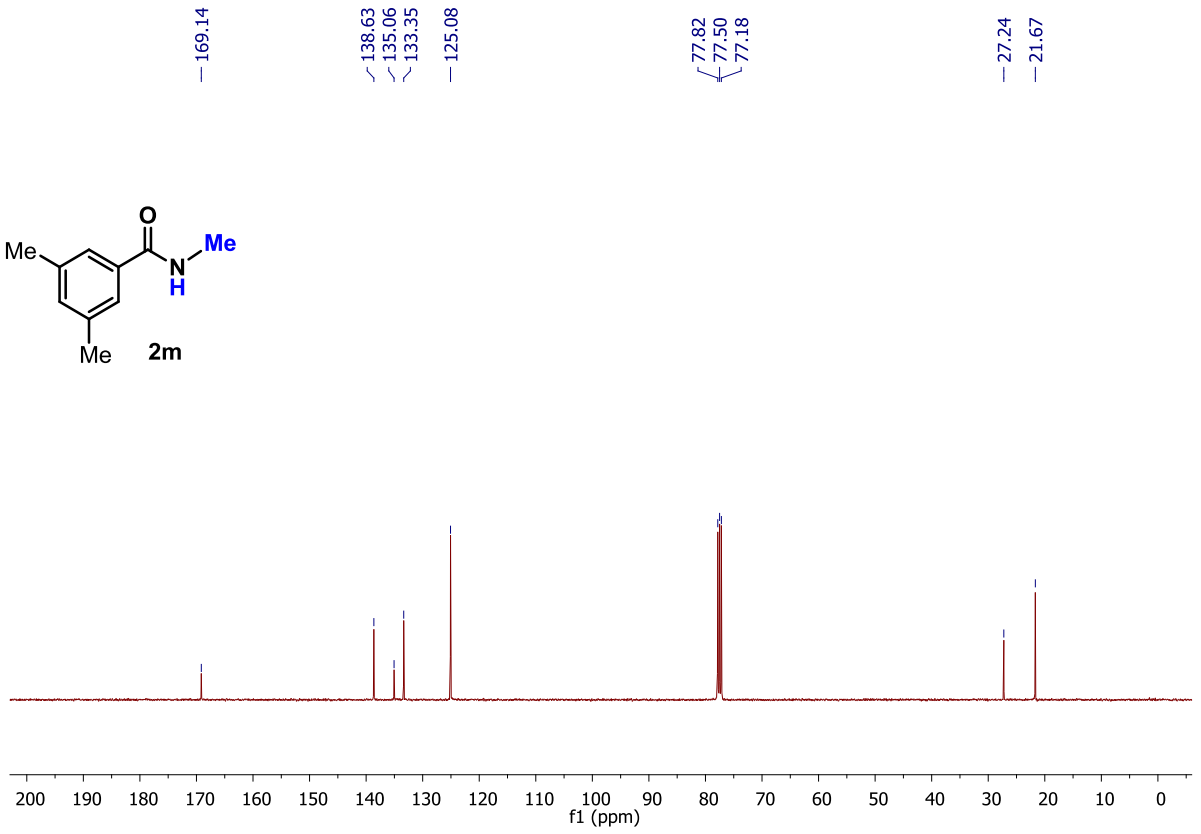
135.03
134.11
131.61
130.98
130.56
128.74
127.75
127.52
126.87
125.88
125.32
125.17
77.82
77.50
77.18
27.31
O
N
H
Me
2l
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Me
O
N
Me
H
Me
2m
7.3348
7.2401
7.0787
6.2632
2.9650
2.9529
2.3038
2.05
1.00
1.00
3.06
6.11
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
f1 (ppm)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138.63
135.06
133.35
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77.82
77.50
77.18
27.24
21.67
Me
O
N
Me
H
Me
2m
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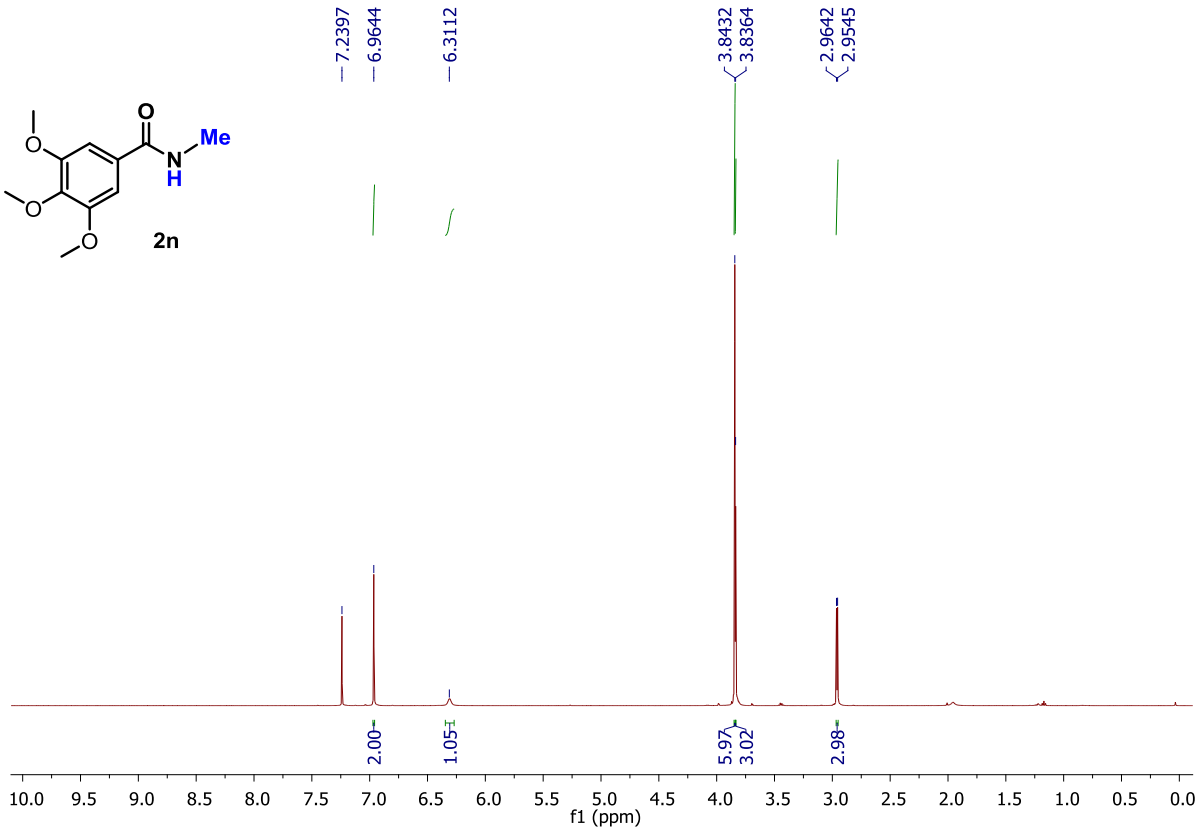
f1 (ppm)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6.9644
6.3112
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3.8364
2.9642
2.9545
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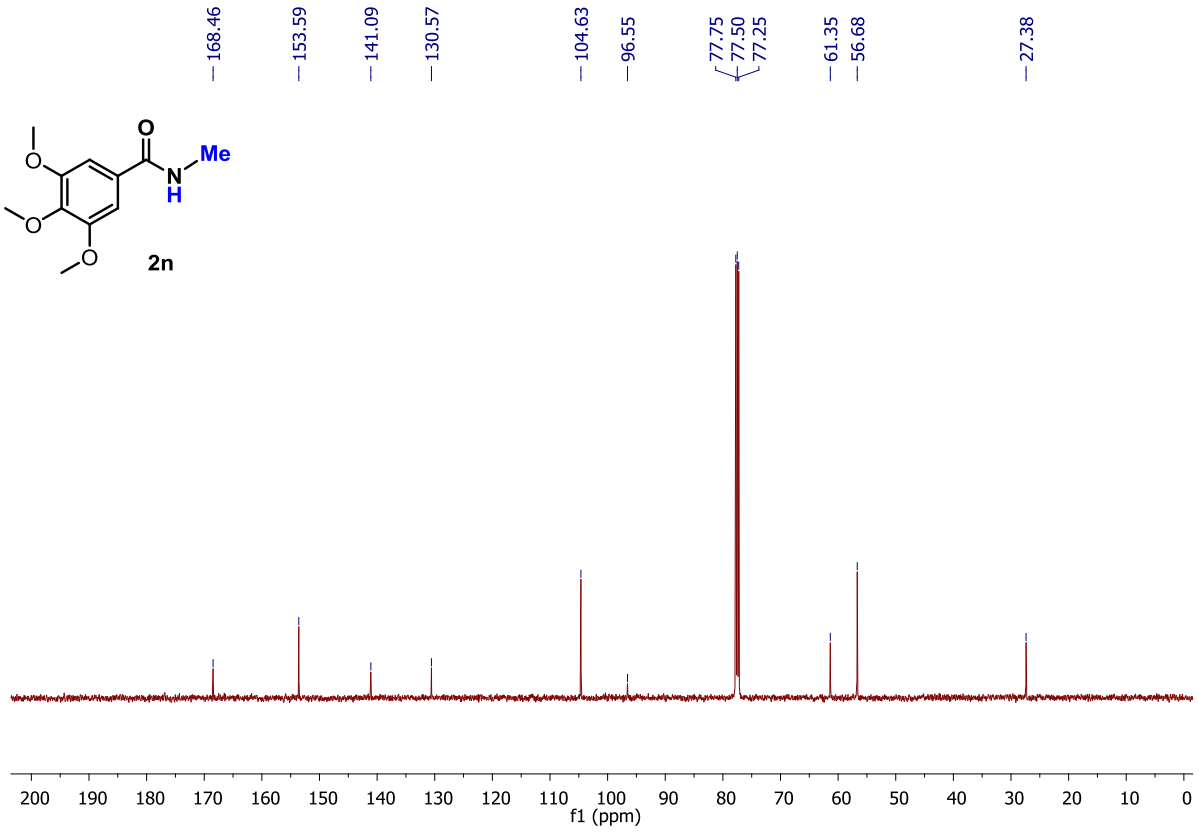
N
H
Me
2n
2.00
1.05
5.97
3.02
2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


168.46
153.59
141.09
130.57
104.63
96.55
77.75
77.50
77.25
61.35
56.68
27.38
O
N
H
Me
2n
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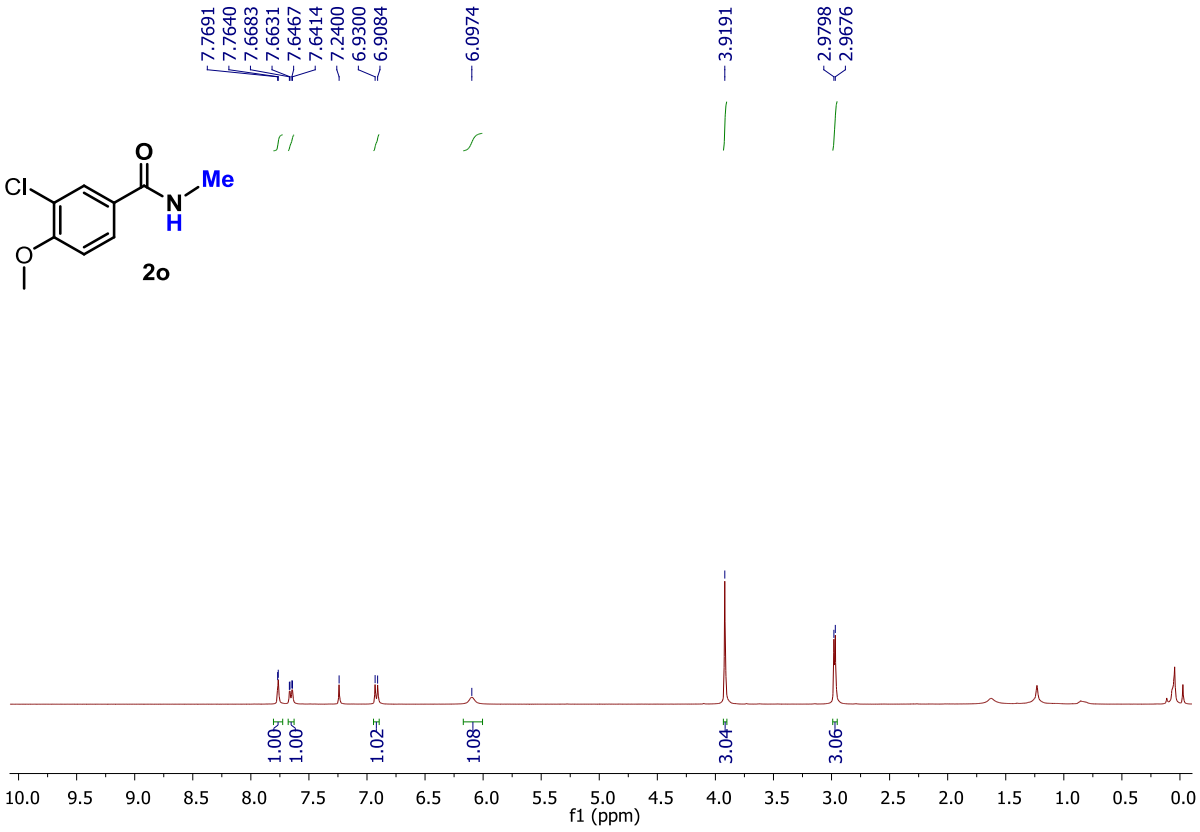
f1 (ppm)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7.6683
7.6631
7.6467
7.6414
7.2400
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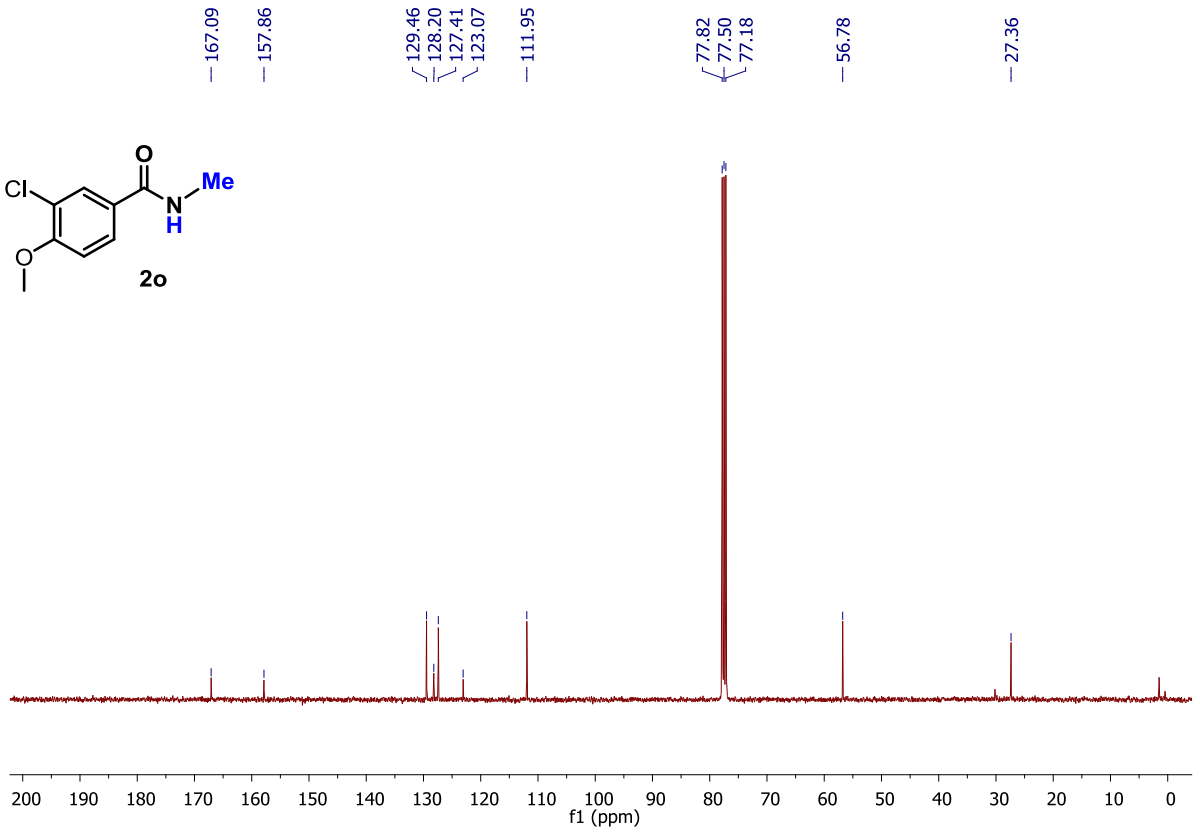
6.9084
6.0974
3.9191
2.9798
2.9676
Cl
O
N
H
Me
O
2o
1.00
1.00
1.02
1.08
3.04
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


167.09
157.86
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128.20
127.41
123.07
111.95
77.82
77.50
77.18
56.78
27.36
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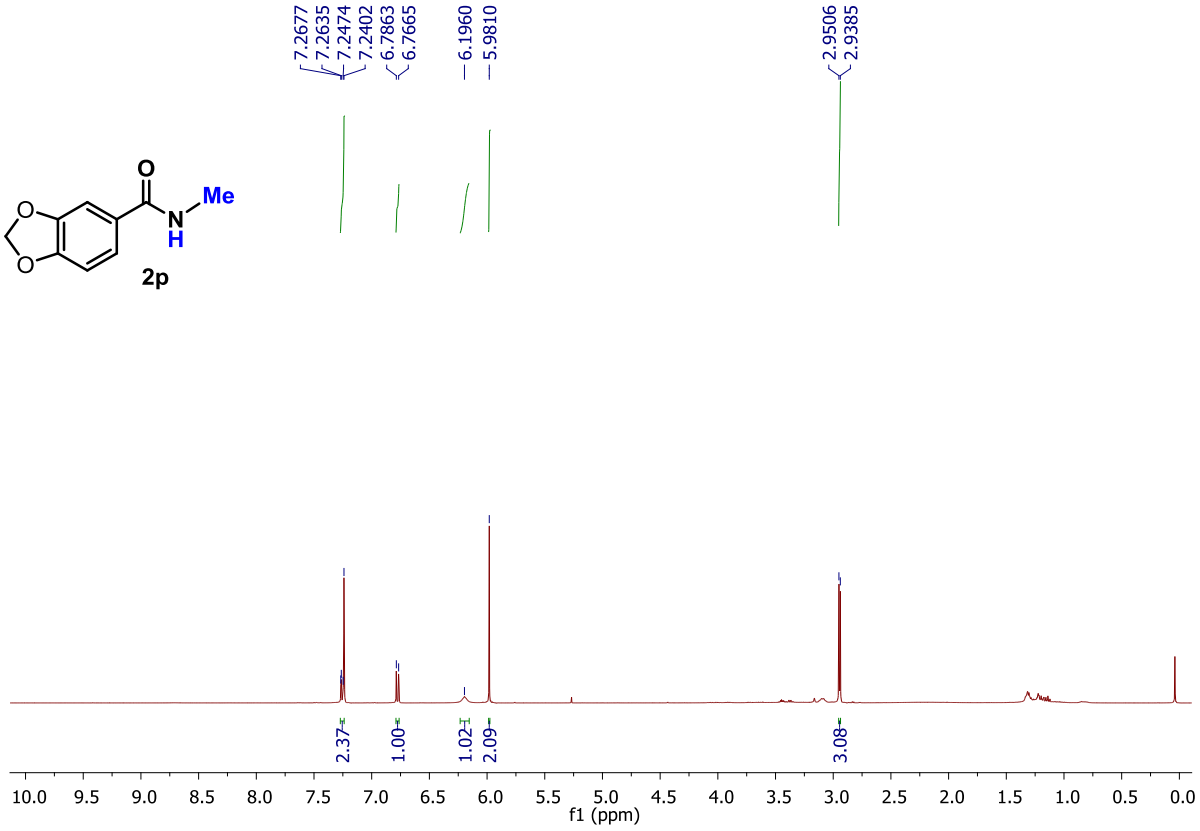
O
N
H
Me
O
2o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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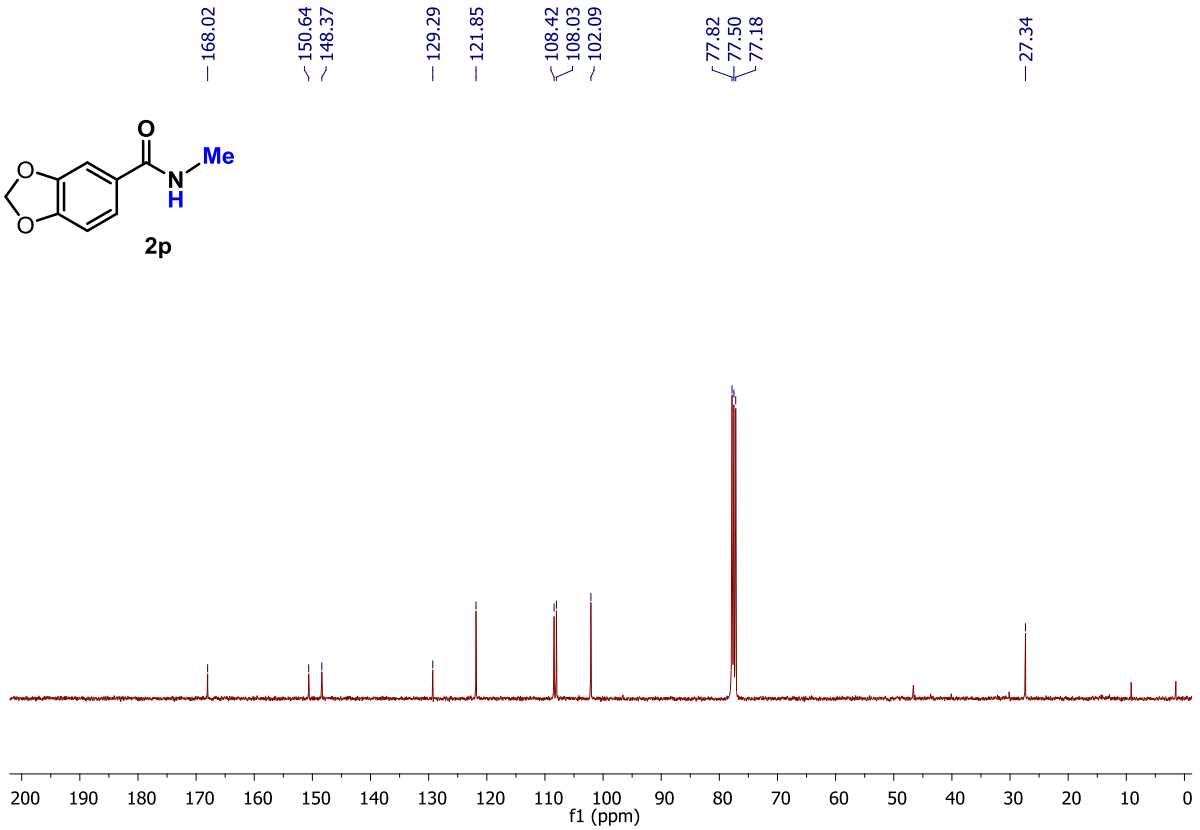
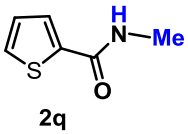
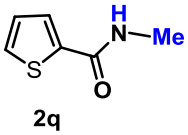
7.2635
7.2474
7.2402
6.7863
6.7665
6.1960
5.9810
2.9506
2.9385
O
Me
N
H
O
O
2p
2.37
1.00
1.02
2.09
3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


168.02
150.64
148.37
129.29
121.85
108.42
108.03
102.09
77.82
77.50
77.18
27.34
O
Me
N
H
O
O
2p
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


H
N
Me
S
O

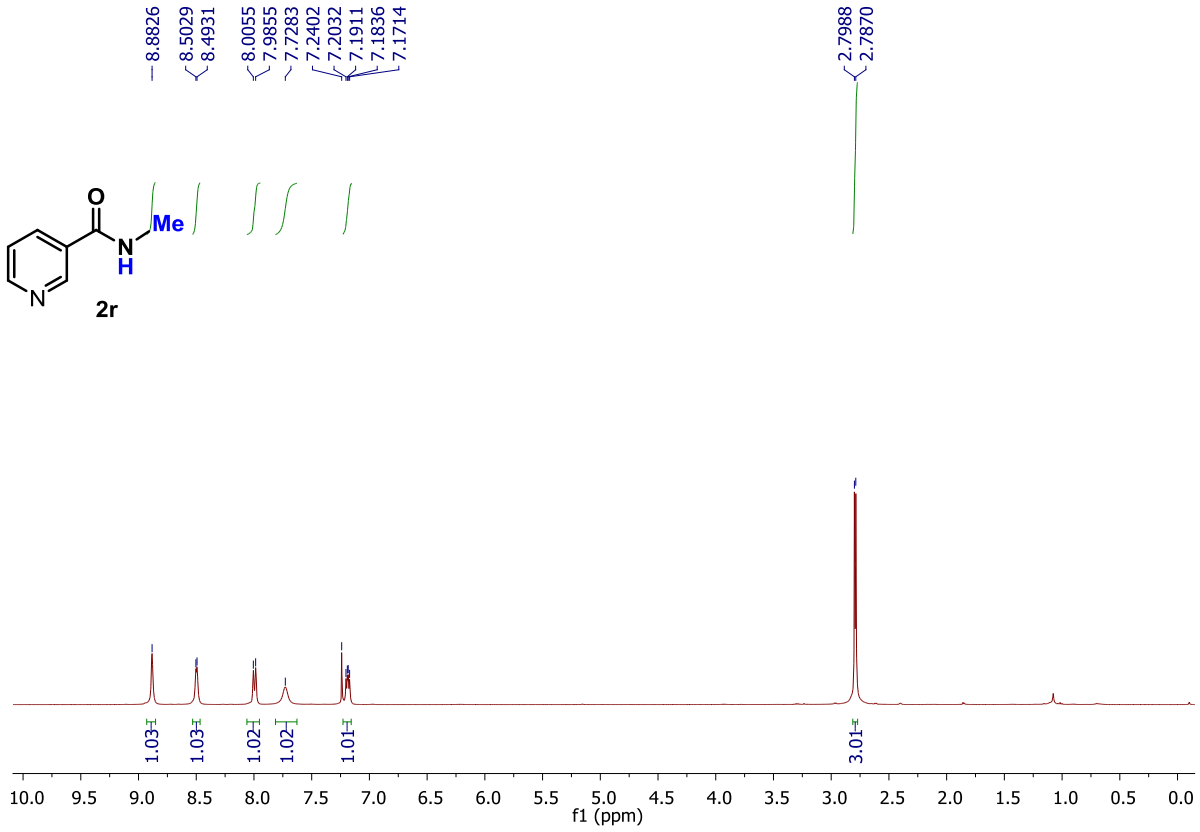
2q

7.5445
7.5357
7.4092
7.3971
7.2402
7.0230
7.0114
7.0011
6.5424
2.9428
1.04
1.00
1.06
0.96
3.08
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
f1 (ppm)


H
N
Me
S
O

2q

163.20
139.47
130.08
128.50
128.07
77.82
77.50
77.18
27.15
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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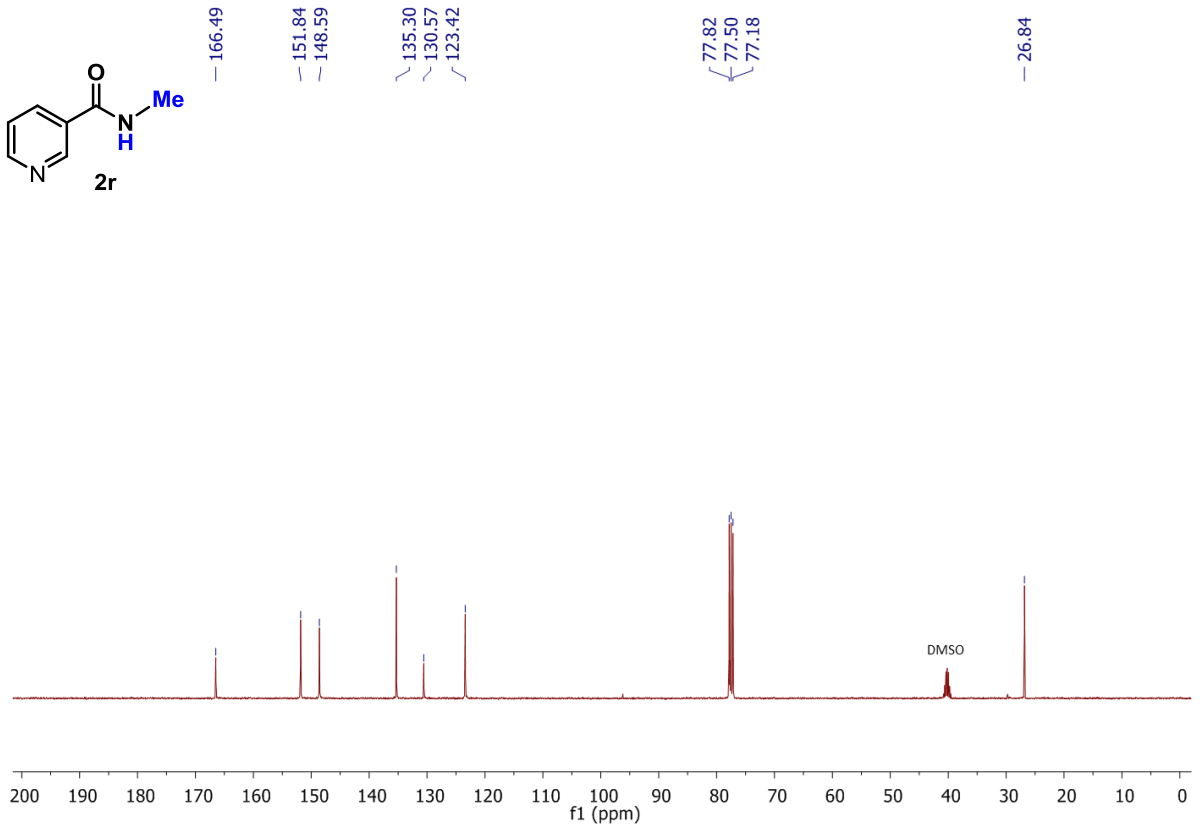
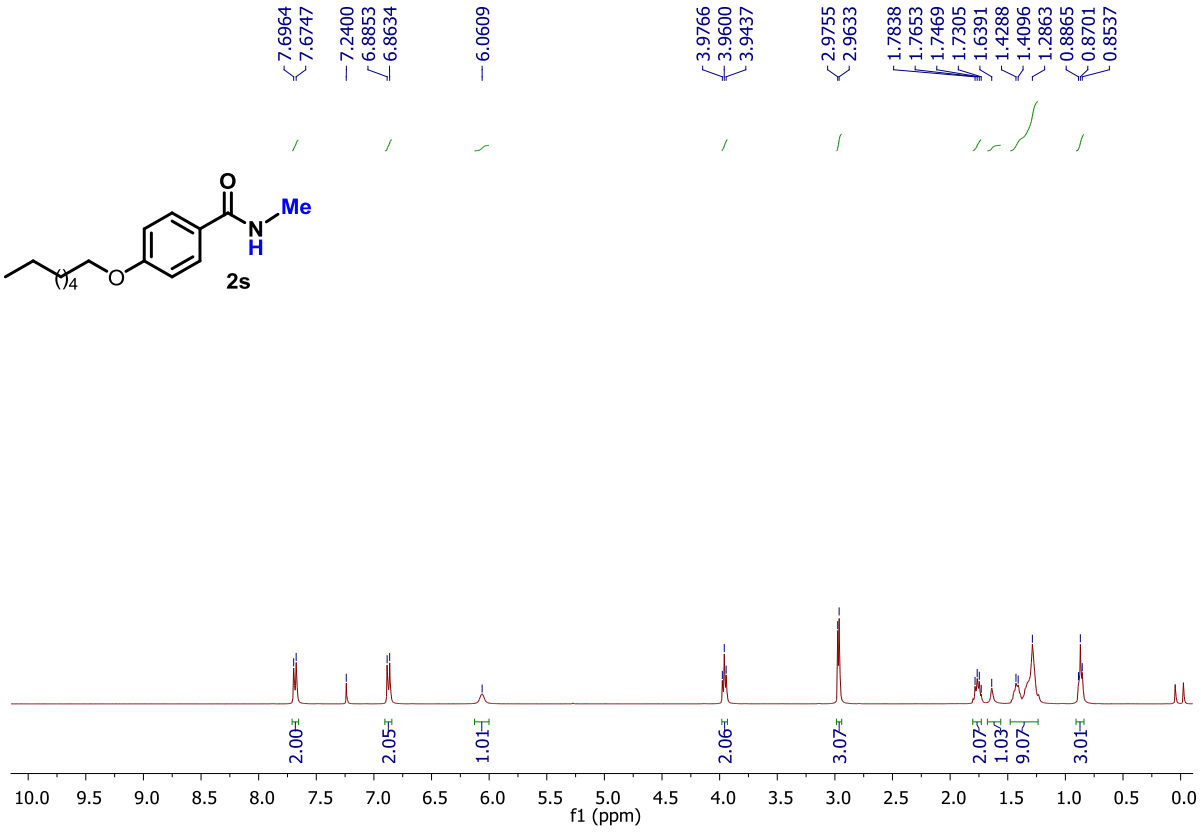
8.5029
8.4931
8.0055
7.9855
7.7283
7.2402
7.2032
7.1911
7.1836
7.1714
2.7988
2.7870
O
N
H
Me
2r
1.03
1.03
1.02
1.02
1.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.49
151.84
148.59
135.30
130.57
123.42
77.82
77.50
77.18
26.84
O
N
H
Me
2r
DMSO
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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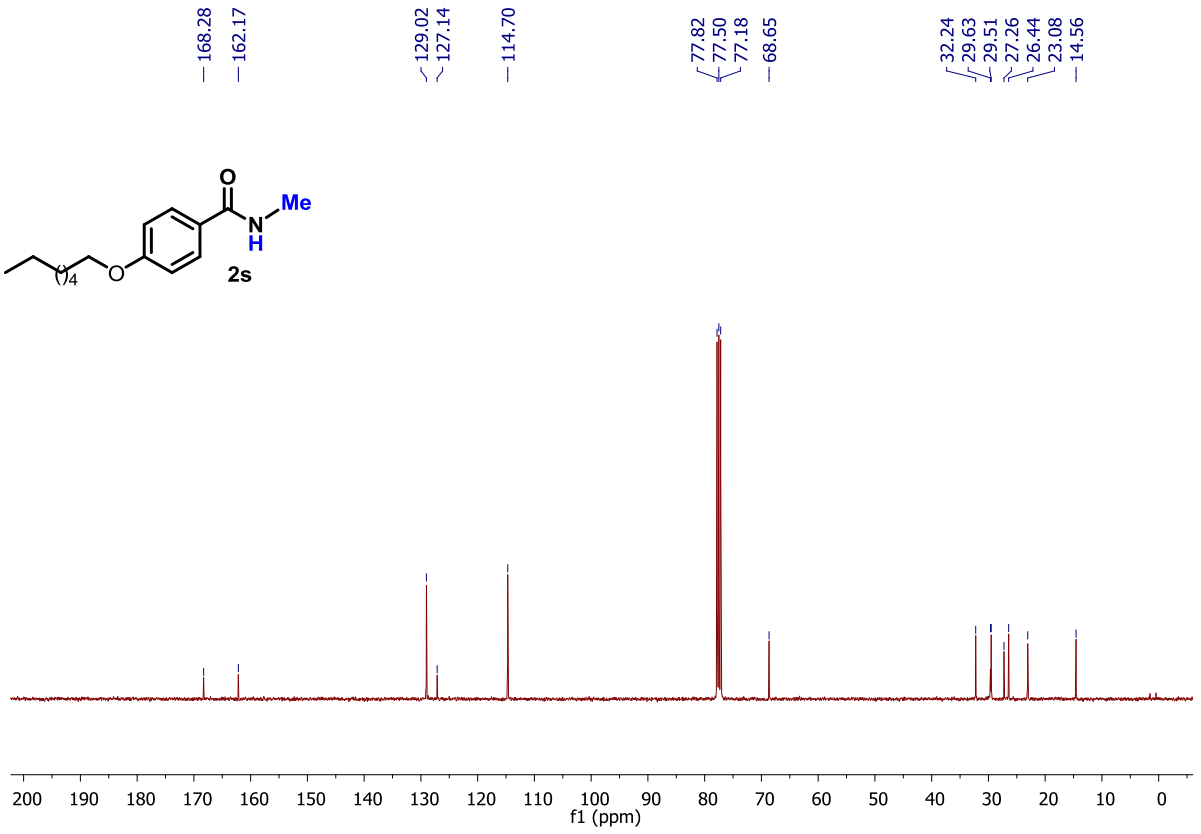
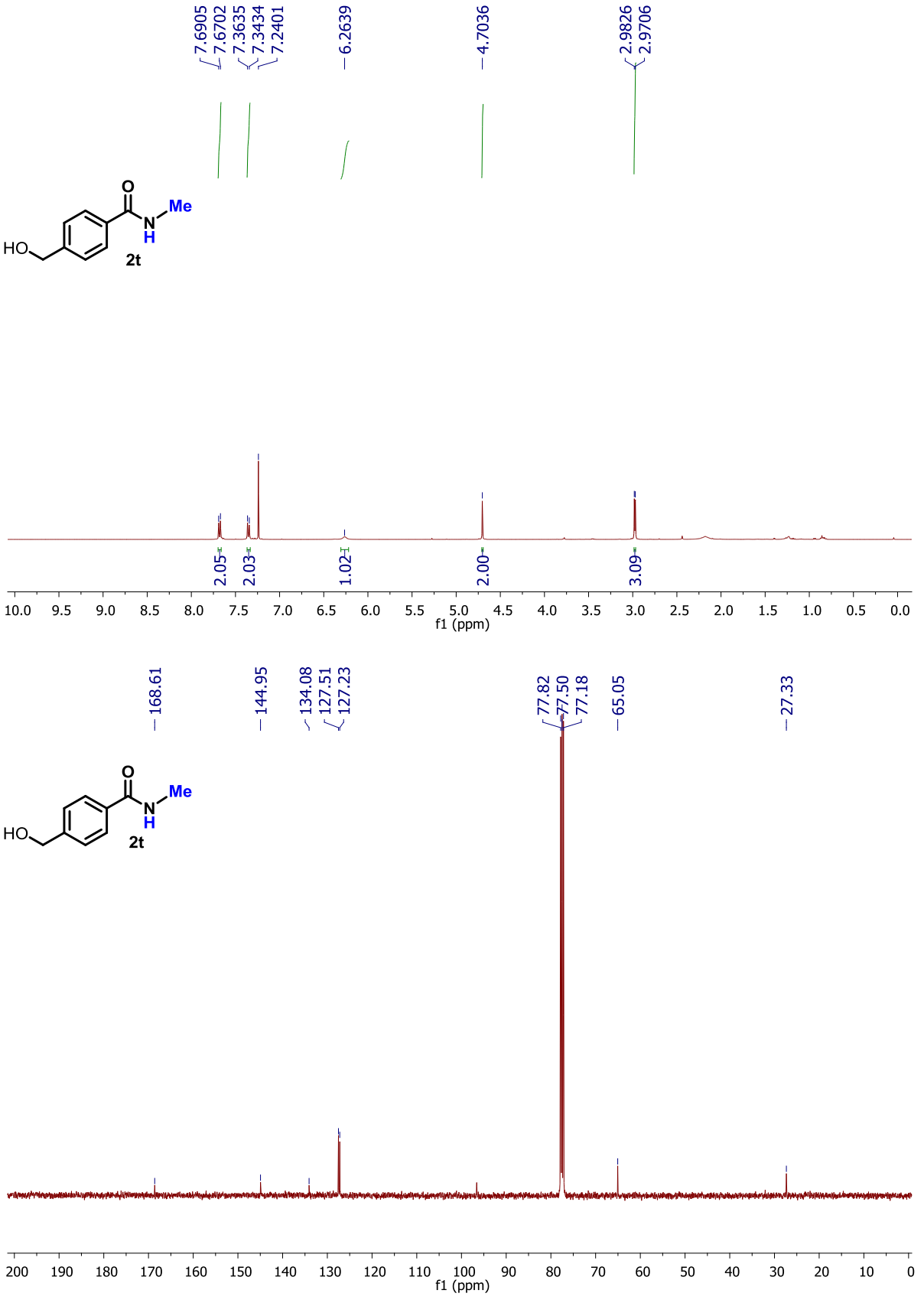
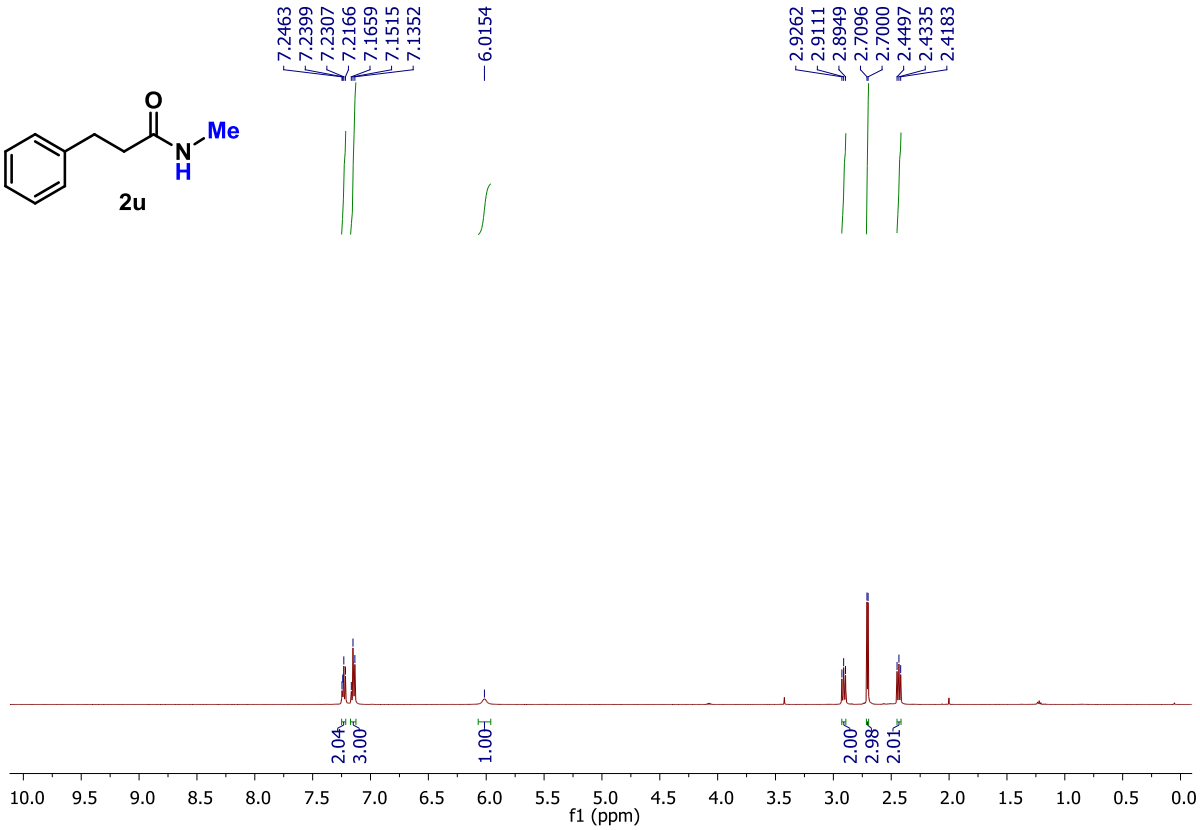
7.6747
7.2400
6.8853
6.8634
6.0609
3.9766
3.9600
3.9437
2.9755
2.9633
1.7838
1.7653
1.7469
1.7305
1.6391
1.4288
1.4096
1.2863
0.8865
0.8701
0.8537
O
N
H
Me
2s
2.00
2.05
1.01
2.06
3.07
2.07
1.03
9.07
3.01
f1 (ppm)


168.28
162.17
129.02
127.14
114.70
77.82
77.50
77.18
68.65
32.24
29.63
29.51
27.26
26.44
23.08
14.56
O
N
H
Me
2s
f1 (ppm)


7.6905
7.6702
7.3635
7.3434
7.2401
6.2639
4.7036
2.9826
2.9706
O
Me
N
H
HO
2t
2.05
2.03
1.02
2.00
3.09
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
f1 (ppm)
168.61
144.95
134.08
127.51
127.23
77.82
77.50
77.18
65.05
27.33
O
Me
N
H
HO
2t
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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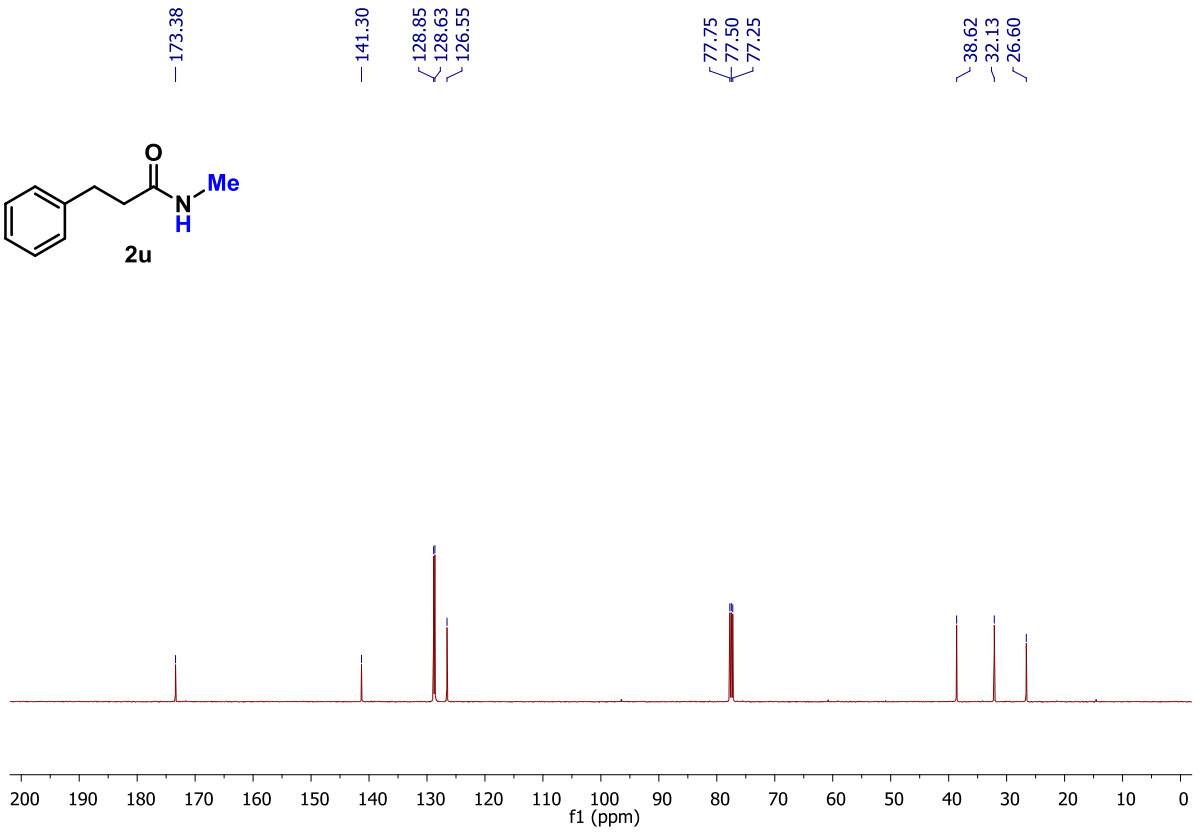
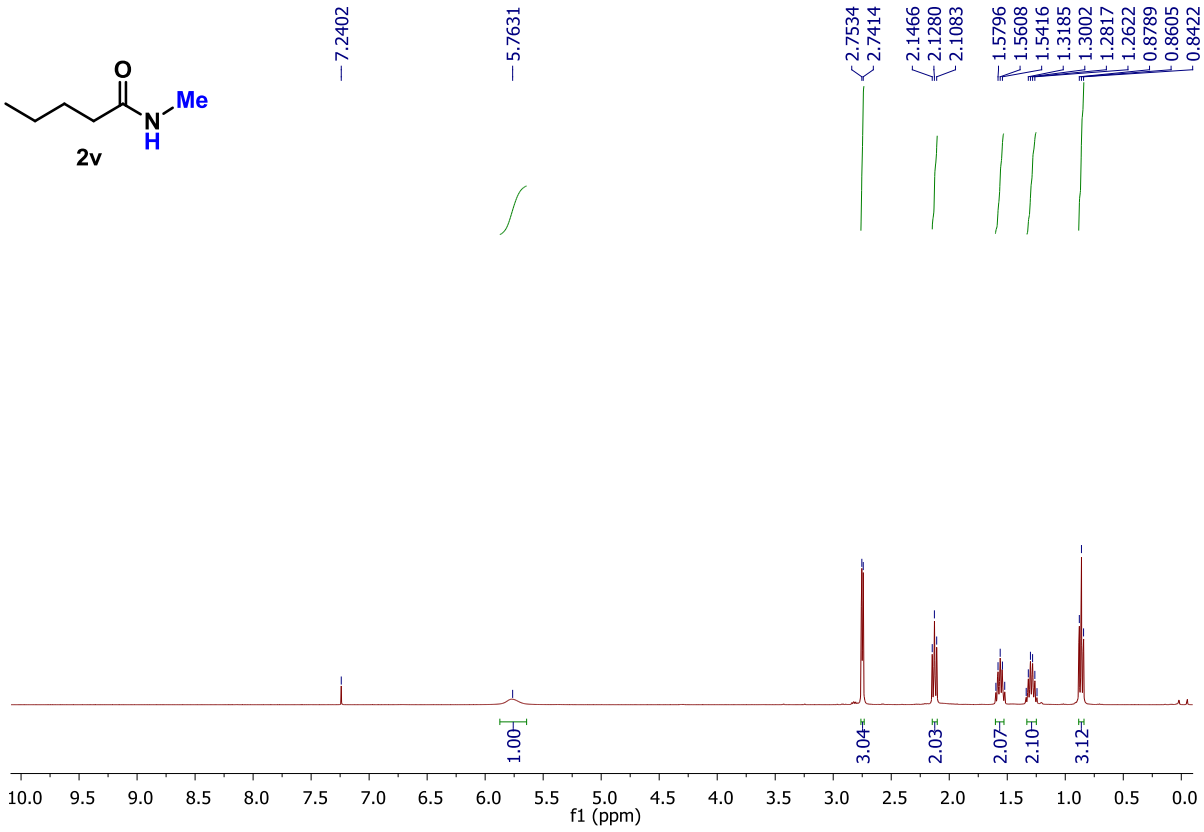
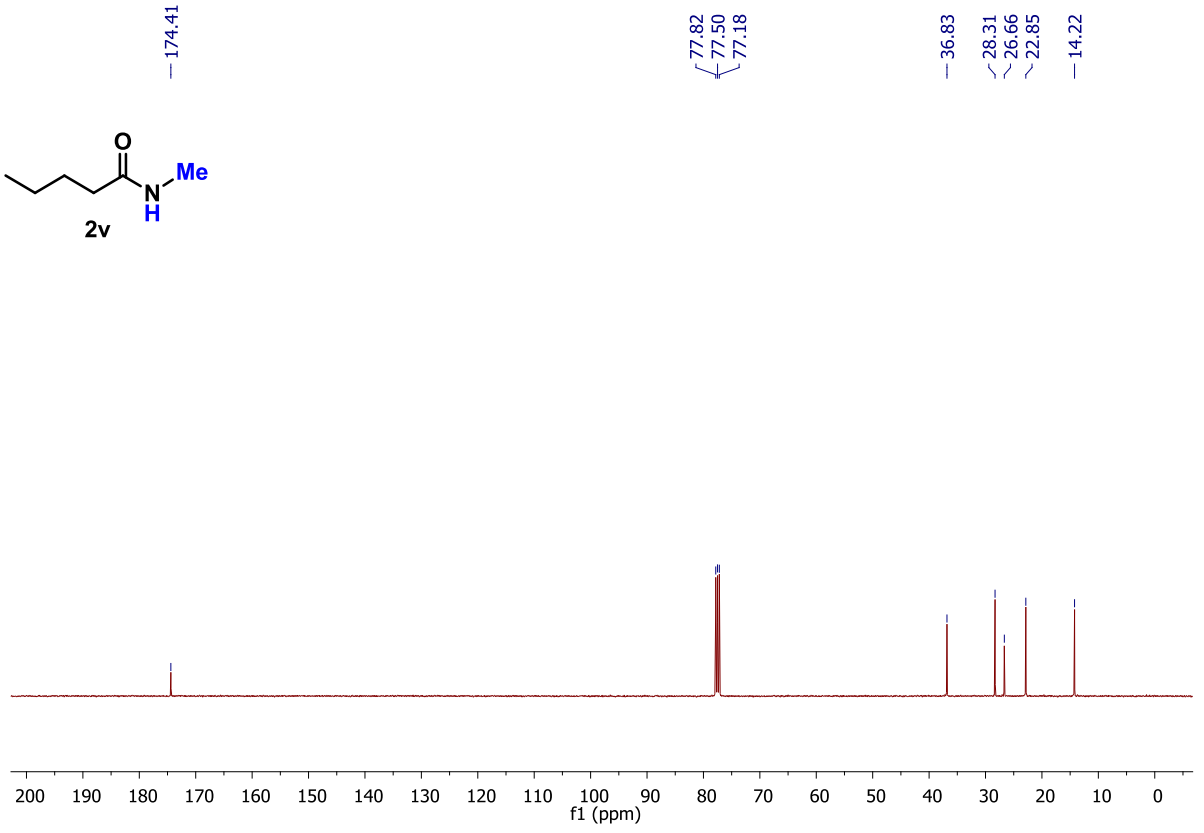
7.2399
7.2307
7.2166
7.1659
7.1515
7.1352
6.0154
2.9262
2.9111
2.8949
2.7096
2.7000
2.4497
2.4335
2.4183
O
N
H
Me
2u
2.04
3.00
1.00
2.00
2.98
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


173.38
141.30
128.85
128.63
126.55
77.75
77.50
77.25
38.62
32.13
26.60
O
N
H
Me
2u
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
Me
N
H
2v
7.2402
5.7631
2.7534
2.7414
2.1466
2.1280
2.1083
1.5796
1.5608
1.5416
1.3185
1.3002
1.2817
1.2622
0.8789
0.8605
0.8422
1.00
3.04
2.03
2.07
2.10
3.12
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
f1 (ppm)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77.82
77.50
77.18
36.83
28.31
26.66
22.85
14.22
O
Me
N
H
2v
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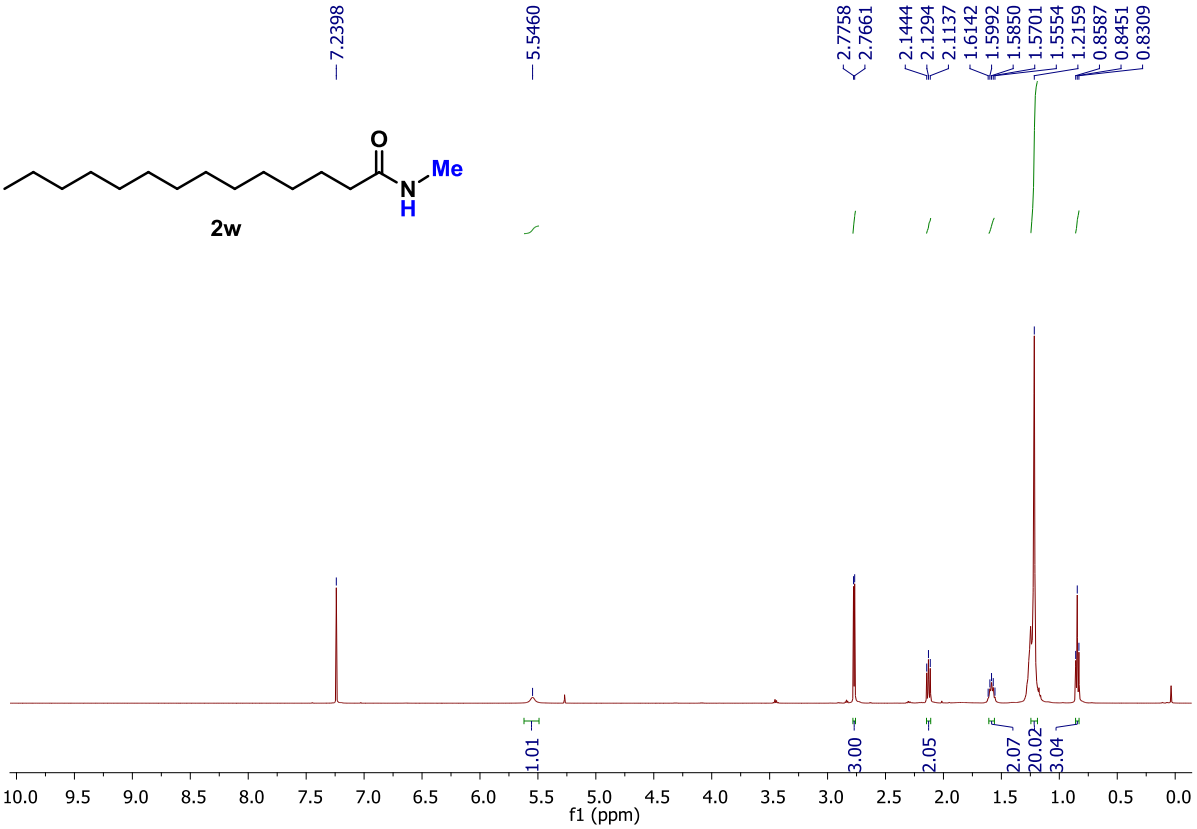
f1 (ppm)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2.7661
2.1444
2.1294
2.1137
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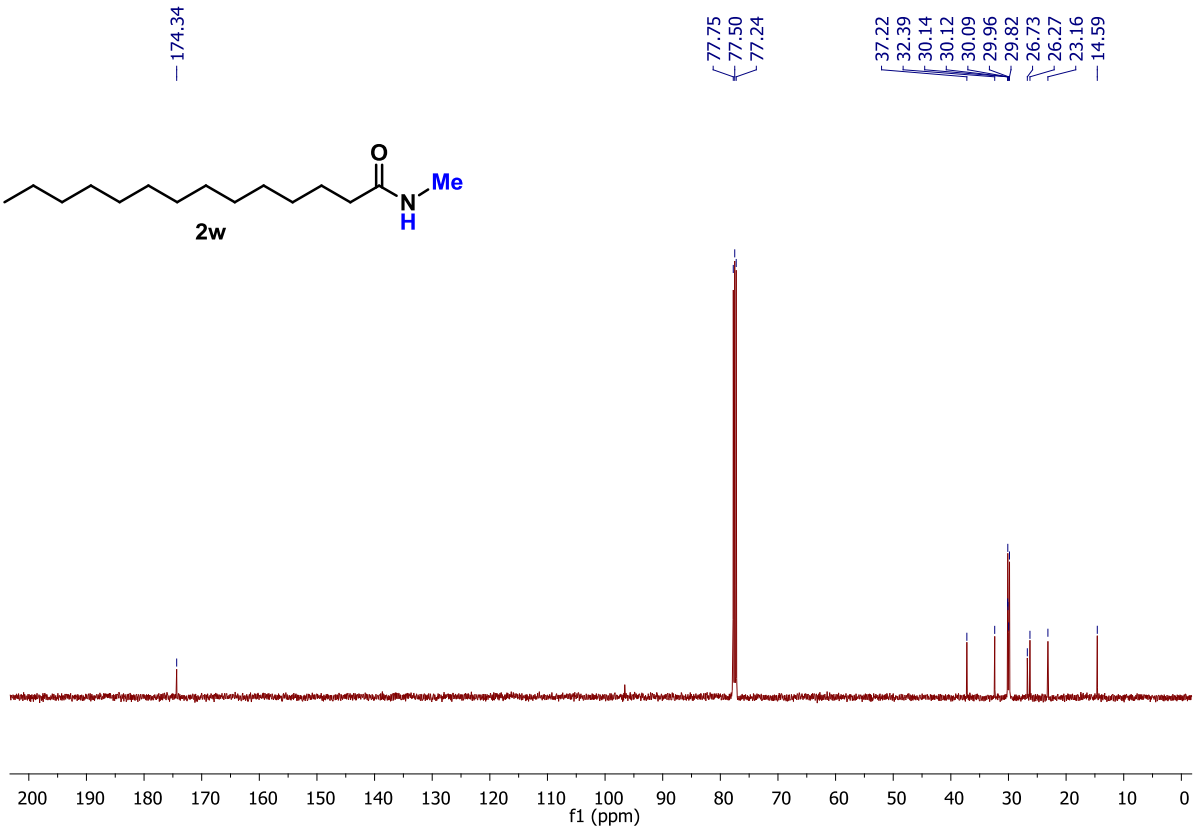
1.5992
1.5850
1.5701
1.5554
1.2159
0.8587
0.8451
0.8309
O
N
H
Me
2w
1.01
3.00
2.05
2.07
20.02
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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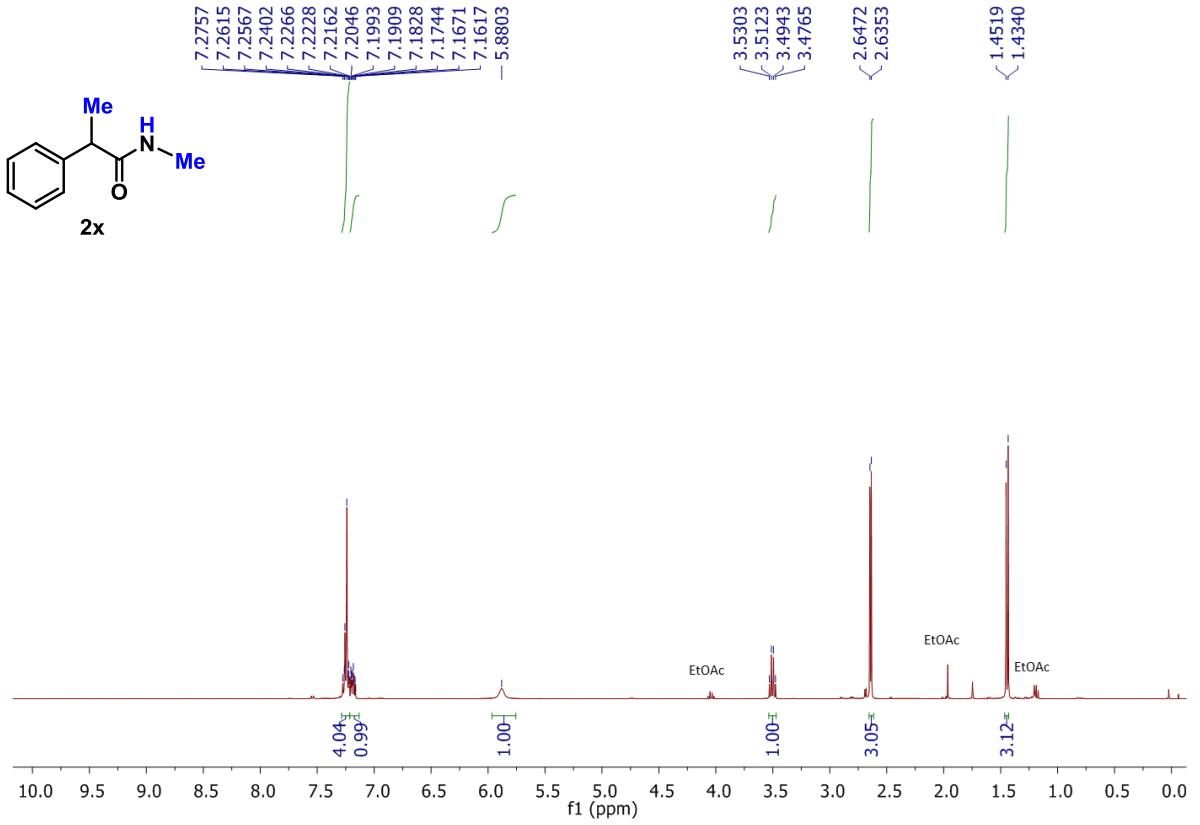
77.75
77.50
77.24
37.22
32.39
30.14
30.12
30.09
29.96
29.82
26.73
26.27
23.16
14.59
O
N
H
Me
2w
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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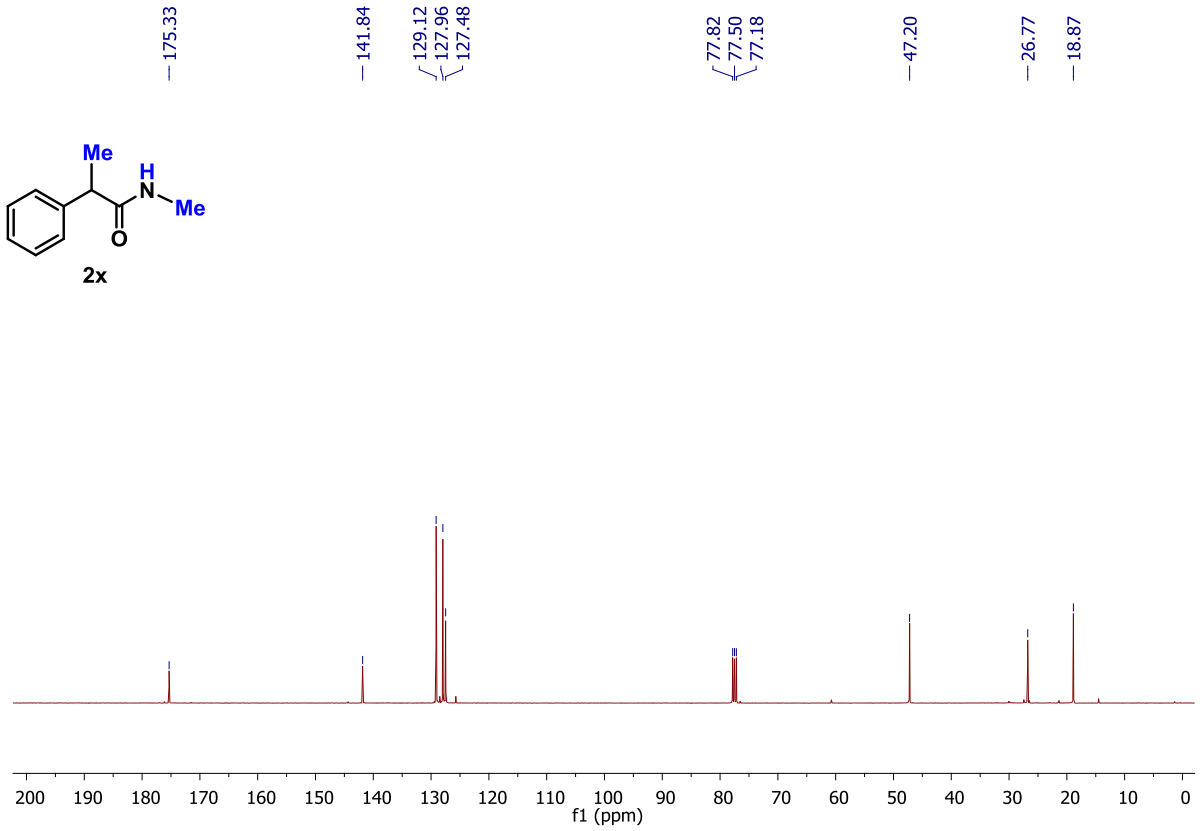
7.2567
7.2402
7.2266
7.2228
7.2162
7.2046
7.1993
7.1909
7.1828
7.1744
7.1671
7.1617
5.8803
3.5303
3.5123
3.4943
3.4765
2.6472
2.6353
1.4519
1.4340
Me
H
N
Me
O
2x
EtOAc
EtOAc
EtOAc
4.04
0.99
1.00
1.00
3.05
3.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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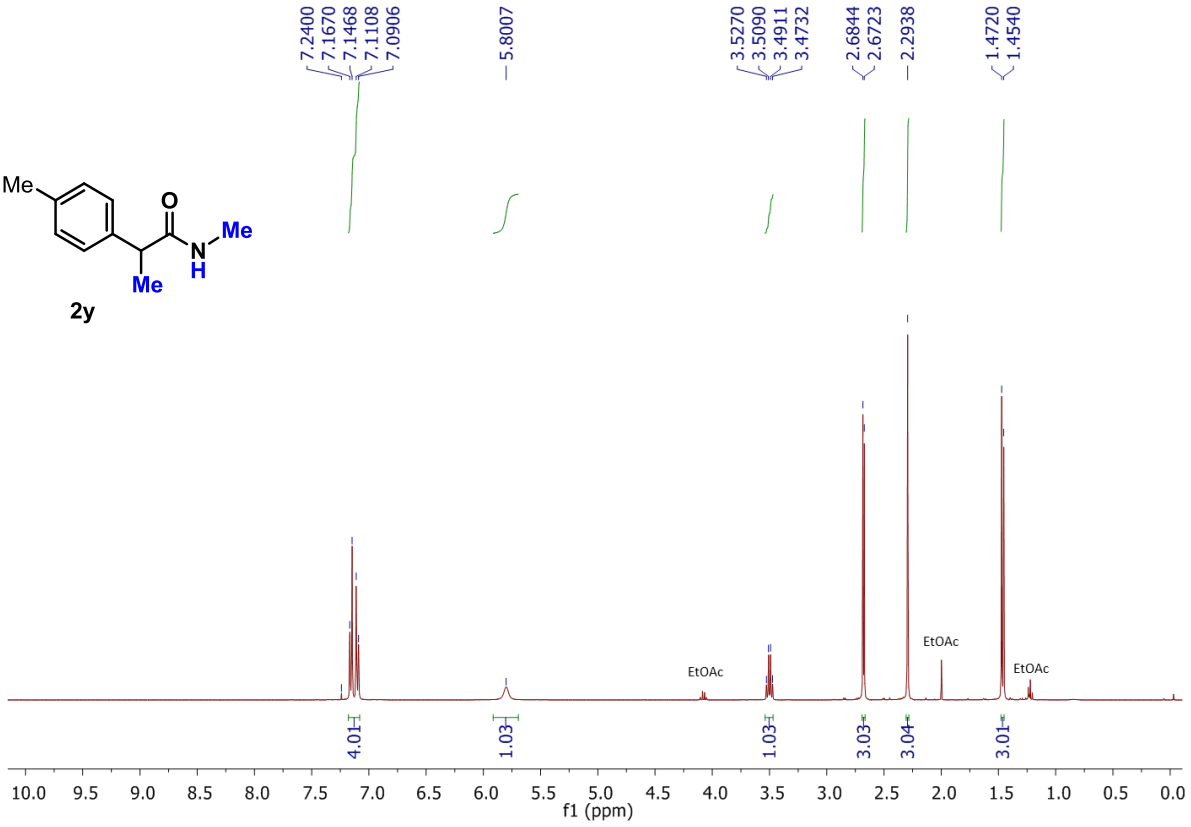
141.84
129.12
127.96
127.48
77.82
77.50
77.18
47.20
26.77
18.87
Me
H
N
Me
O
2x
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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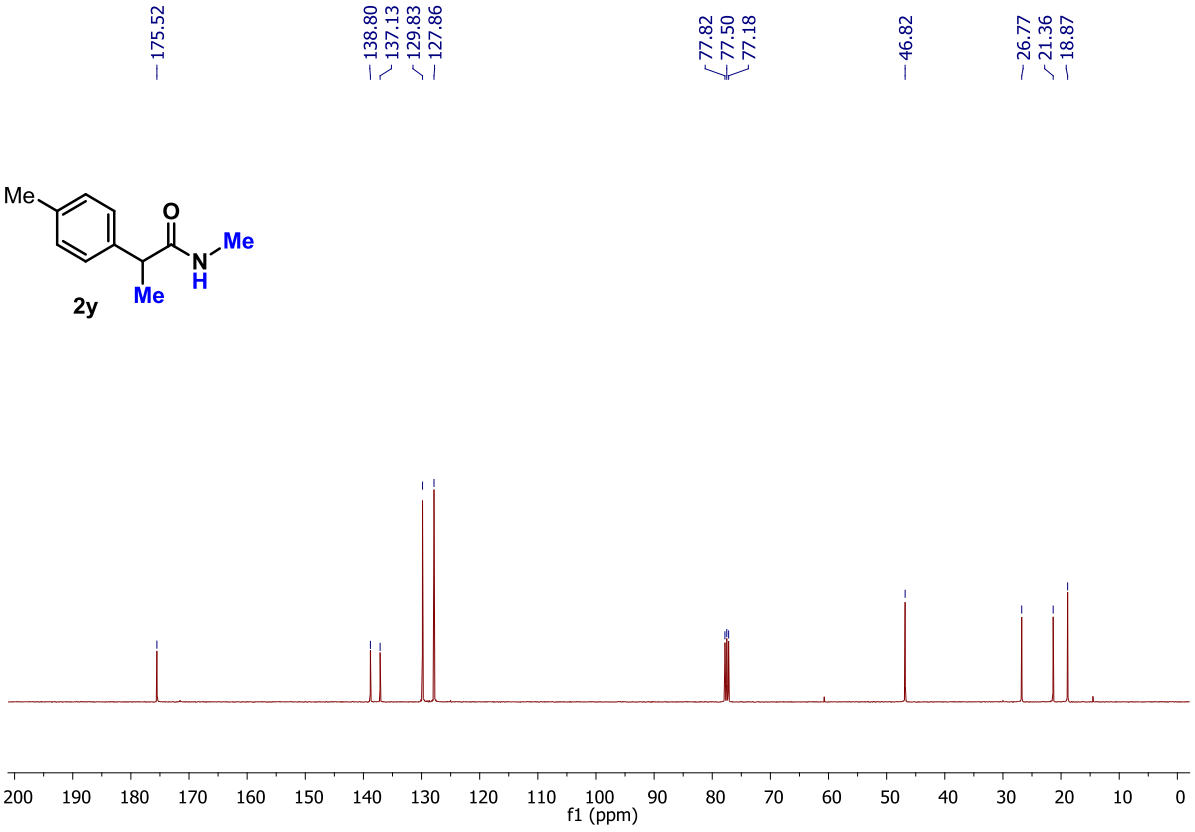
7.1108
7.0906
5.8007
3.5270
3.5090
3.4911
3.4732
2.6844
2.6723
2.2938
1.4720
1.4540
Me
O
N
H
Me
Me
2y
EtOAc
EtOAc
EtOAc
4.01
1.03
1.03
3.03
3.04
3.01
f1 (ppm)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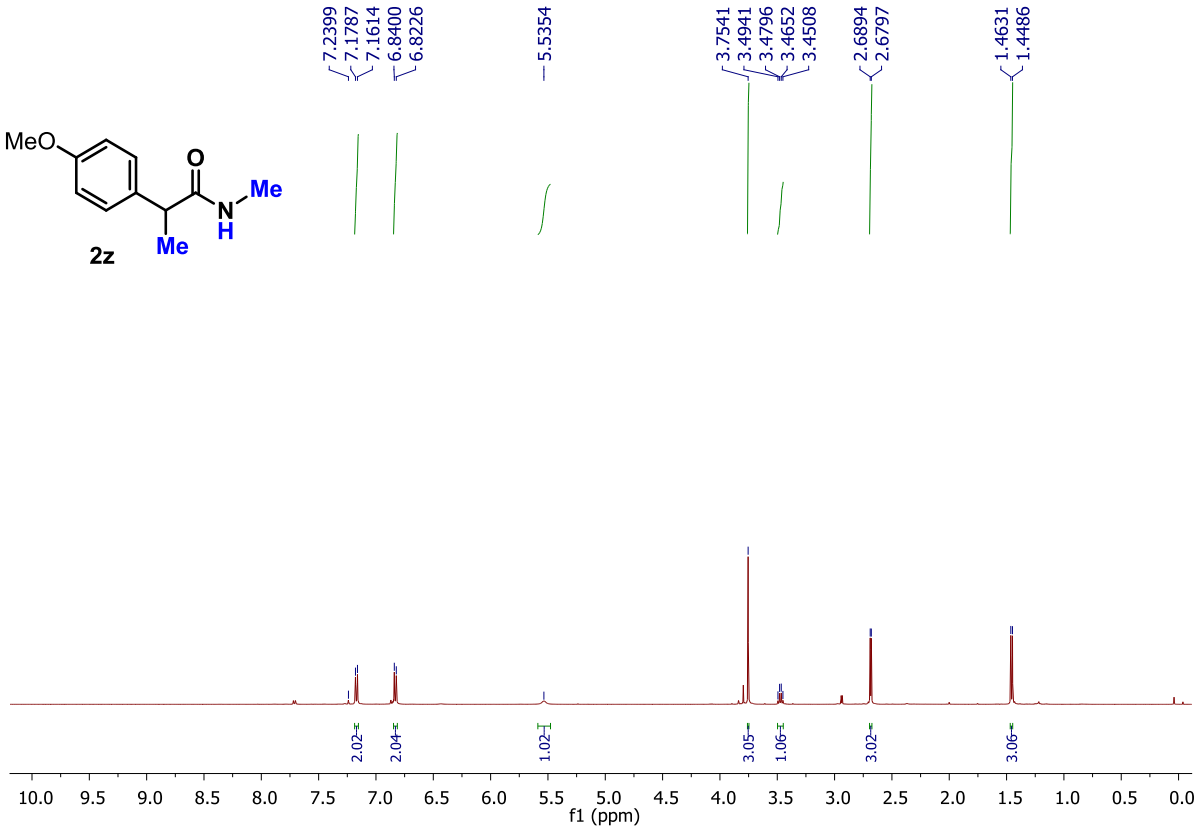
138.80
137.13
129.83
127.86
77.82
77.50
77.18
46.82
26.77
21.36
18.87
Me
O
N
H
Me
Me
2y
f1 (ppm)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7.1614
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6.8226
5.5354
3.7541
3.4941
3.4796
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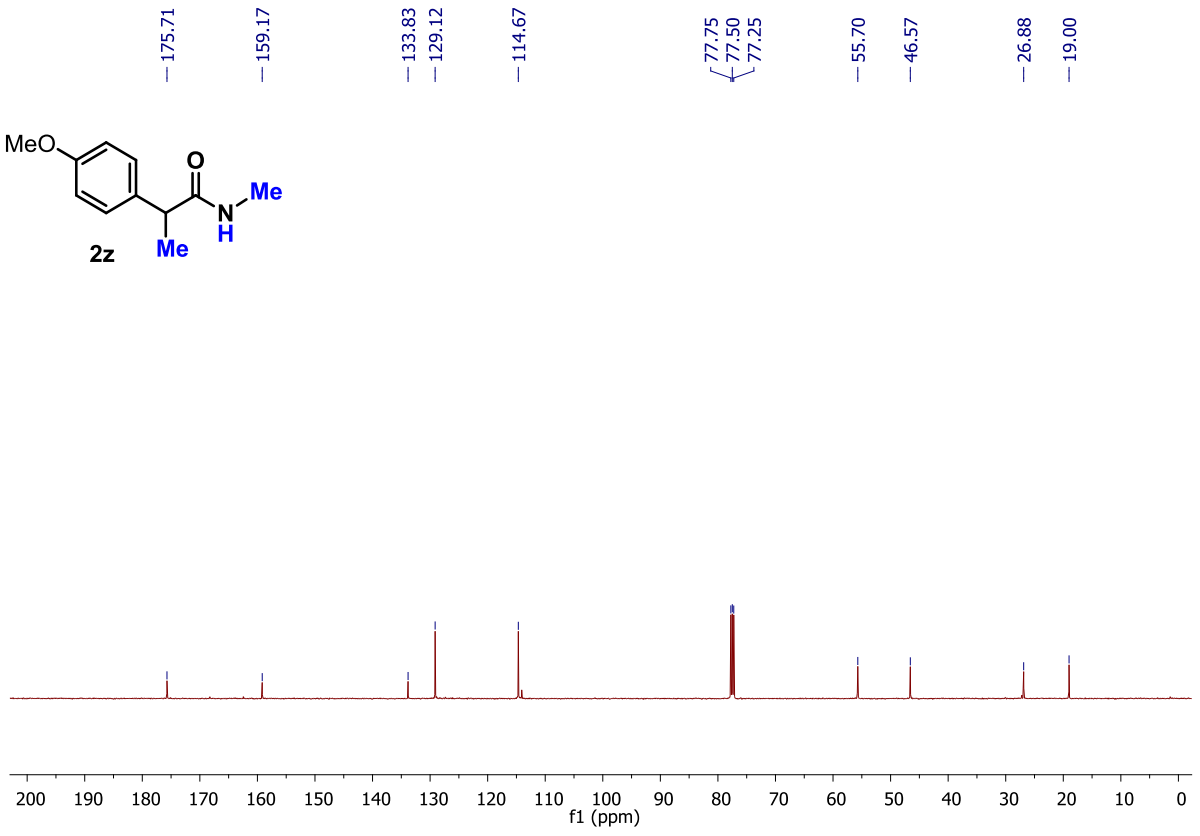
3.4508
2.6894
2.6797
1.4631
1.4486
MeO
O
N
H
Me
Me
2z
2.02
2.04
1.02
3.05
1.06
3.02
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.12
114.67
77.75
77.50
77.25
55.70
46.57
26.88
19.00
MeO
O
N
H
Me
Me
2z
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

14. References

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