

Nitrogen-to-functionalized carbon atom transmutation of pyridine

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1. General information

1.1 General remarks

All reagents were purchased from Alfa Aesar, Sigma-Aldrich, Merck, TCI, Fluorochem, Combi-blocks, VWR and used without further purification, except otherwise stated. All the solvents were bought from Acros in AcroSeal® bottles and were directly stored under 3 or 4 Å molecular sieves, replacing the collected volume with argon. All reactions were carried out in an oven-dried glassware under an atmosphere of argon using standard Schlenk technique, unless otherwise noted. Solvents for chromatographic purification (pentane, EtOAc, dichloromethane and methanol) were purchased as technical grade and purified by atmospheric pressure distillation. Reaction temperatures are referred to the temperature of the heating medium, unless otherwise stated.

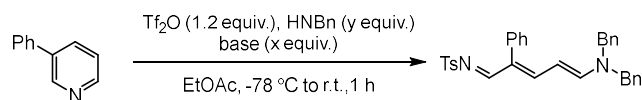
1.2 Analytical techniques and compound purification

NMR-spectra were recorded on a Bruker Avance II 300, Avance II 400, Agilent DD2 500 or DD2 600 spectrometers. All spectral data was acquired at 295 K, except otherwise stated. Deuterated solvents were purchased from Eurisotop (CDCl₃, deuteration > 99.8%). ¹H and ¹³C chemical shifts (δ) are quoted in parts per million (ppm) against tetramethylsilane (TMS, δ = 0.00 ppm) and were internally referenced to residual CHCl₃ (7.26 ppm for ¹H, 77.0 ppm for ¹³C). Coupling constants (J) are reported in Hertz (Hz) to the nearest 0.1 Hz. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, m = multiplet. High-resolution mass spectra (HRMS) were obtained by the MS service of the Organisch-Chemisches Institut, Universität Münster, using electrospray ionisation (ESI) on a Bruker Daltonics, MicroToF spectrometer and calibrated using formate ion clusters. Thin layer chromatography was carried out on Merck silica gel 60 F254 pre-coated aluminium sheets and were visualized using UV light (254 nm) and stained with basic aqueous potassium permanganate. Flash chromatography was carried out using silica gel (Acros Organics, 0.035-0.070 mm, 60 Å) under a light positive pressure of argon, eluting with the specified solvent system as mentioned.

2. Reaction development

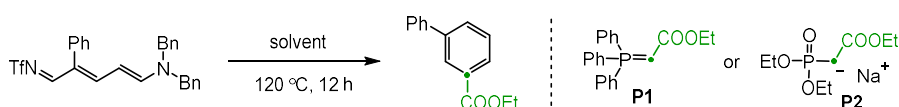
2.1 Optimization of the reaction conditions

Table 1. Ring open of pyridine.



Entry	Base	x	y	RSM (%)	Yield (%)
1	Collidine	1.0	1.2	15	82
2	NaHCO ₃	1.0	1.2	75	22
3	K ₂ CO ₃	1.0	1.2	43	30
4	NaO ^t Bu	1.0	1.2	37	56
5	KO ^t Bu	1.0	1.2	26	57
6	KO ^t Bu	1.0	1.0	21	71
7	KO ^t Bu	1.2	1.2	12	80

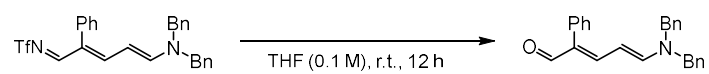
Table 2. Screening of solvent for N-to-C from zincke-imine



entry	solvent	reagent	yield (%)
1	Toluene	P1	14
2	CH ₂ Cl ₂	P1	trace
3	THF	P1	trace
4	DMF	P1	trace
5	EtOAc	P1	9
6	CH ₃ CN	P1	0
7	EtOH	P1	0
8	Toluene (r.t.)	P1	trace
9	CH ₂ Cl ₂	P2	20
10	THF	P2	22

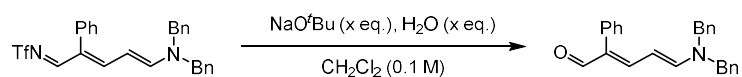
Reaction conditions: Zincke imine (0.05 mmol), **P1** (1.5 eq.) or **P2** (1.5 eq., prepared from ethyl 2-(diethoxyphosphoryl)acetate and NaH), stirred at 120 °C for 12 h.

Table 3. Screening of conditions for hydrolysis step



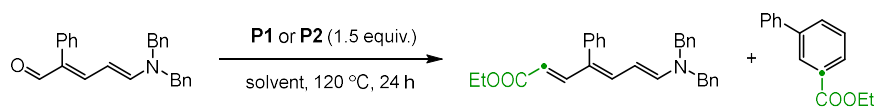
Entry	Conditions	RSM (%)	Yield (%)
1	HCl (1 M)	100	0
2	NaOH (1 M)	100	0
3	Silic gel (50 mg/mL)	100	0
4	NaOH/MeOH (1:1, 1 M)	0	0
5	110 °C instead of r.t.	100	0
6	NaO ^t Bu (1.0 equiv.), 120 °C	0	0
7	NaO ^t Bu (2.0 equiv.), H ₂ O (1.0 equiv.) 120 °C	0	99

Table 4. Screening of amount of base, temperature, and time for hydrolysis step



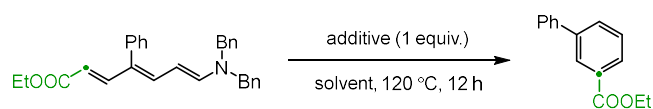
Entry	X (equiv.)	Temperature	Time	Yield (%)
1	2.0	120	15 min	99
2	1.5	120	15 min	99
3	1.2	120	15 min	95
4	1.0	120	15 min	99
9	2.0	r.t.	24 h	98

Table 5. Screening of olefination reagent



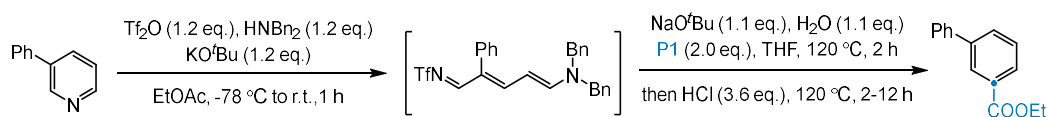
Entry	Reagent	Solvent	RSM	Alkene	Yield (%)
1	P2	THF	5	86	4
2	P2	THF/DCM	29	40	9
3	P2	DCM	48	6	14
4	P2 (140 °C)	DCM	64	4	17
5	P2 (2.0 eq.)	THF	0	94	4
6	P1	DCM	74	17	9

Table 6. Screening of additives for ring closure step



Entry	Additive	solvent	Temp. (°C)	RSM (%)	Yield (%)
1	-	THF	120	30	64
2	NaO ^t Bu	THF	120	96	4
3	AcOH	THF	120	52	41
4	HCl (cat)	THF	120	4	94
5	TFA	Toluene	120	0	34
6	-	Toluene	120	31	58
7	-	CH ₂ Cl ₂	120	0	86
8	-	EtOAc	120	49	44

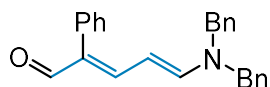
2.2. General procedure for the pyridine-to-benzene reactions



To an oven-dried 10 mL Schlenk tube equipped with a PTFE-coated oval stirring bar was evacuated and re-filled with argon four times, then the vessel was charged with the heterocycle (0.2 mmol) under an argon atmosphere. EtOAc (2 mL, 0.1 M) was added, the reaction vessel cooled to $-78\text{ }^\circ\text{C}$ and Tf_2O (41 μL , 1.2 equiv.) was added dropwise over 5 minutes. The reaction was stirred for 30 minutes before dibenzylamine (46 μL , 1.2 equiv.) was added dropwise as a solution (1.0 M in EtOAc) followed by KO^tBu (27 mg, 1.2 equiv.). The reaction was stirred for a further 30 minutes at $-78\text{ }^\circ\text{C}$. The cooling bath was removed and the reaction was allowed to warm to room temperature while stirring for approximately 30 minutes. The mixture filter over a short plug of silica (1 cm) and the volatiles were removed under reduced pressure to give crude Zincke imines.

A new 10 mL Schlenk tube equipped with a PTFE-coated oval stirring bar was charged with NaO^tBu (21.1 mg, 1.1 equiv.), H_2O (4 μL , 1.1 equiv.) and THF (1 mL, 0.2 M). The crude Zincke imines was added as a solution (0.2 M in THF, 1 mL) and the reaction was stirred 10 minutes at $120\text{ }^\circ\text{C}$. After cooling, phosphonate carbanion (2.0 equiv., the phosphonate carbanion reagent prepared from ethyl 2-(diethoxyphosphoryl)acetate (2.0 equiv.) and NaH (2.5 equiv.) in THF (1 mL) at $0\text{ }^\circ\text{C}$.) was added as a solution (1 mL, 0.4 M in THF), and the reaction continued for an additional 2 hours at $120\text{ }^\circ\text{C}$. Upon cooling to room temperature once again, HCl (180 μL , 3.6 equiv., 4 M in dioxane) was added, and the reaction was stirred for an additional 2 hours at $120\text{ }^\circ\text{C}$. After reaction complete, the resulting solution was transferred to a 25 mL round bottom flask and volatiles were removed under reduced pressure. Purification by flash column chromatography on SiO_2 (pentane/ EtOAc) afforded the corresponding products.

3. Experimental data for the described substances

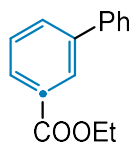


5-(Dibenzylamino)-2-phenylpenta-2,4-dienal (**2a**)

To an oven-dried 10 mL Schlenk tube equipped with a PTFE-coated oval stirring bar was evacuated and re-filled with argon four times, then the vessel was charged with the heterocycle (0.2 mmol) under an argon atmosphere. EtOAc (2 mL, 0.1 M) was added, the reaction vessel cooled to $-78\text{ }^{\circ}\text{C}$ and Ti_2O (41 μL , 1.2 equiv.) was added dropwise over 5 minutes. The reaction was stirred for 30 minutes before dibenzylamine (46 μL , 1.2 equiv.) was added dropwise as a solution (1.0 M in EtOAc) followed by KO^tBu (27 mg, 1.2 equiv.). The reaction was stirred for a further 30 minutes at $-78\text{ }^{\circ}\text{C}$. The cooling bath was removed and the reaction was allowed to warm to room temperature while stirring for approximately 30 minutes. The mixture filter over a short plug of silica (1 cm) and the volatiles were removed under reduced pressure to give crude Zincke imines. A new 10 mL Schlenk tube equipped with a PTFE-coated oval stirring bar was charged with NaO^tBu (21.1 mg, 1.1 equiv.), H_2O (4 μL , 1.1 equiv.) and THF (1 mL, 0.2 M). The crude Zincke imines was added as a solution (0.2 M in THF, 1 mL) and the reaction was stirred 10 minutes at $120\text{ }^{\circ}\text{C}$. After reaction complete, the resulting solution was transferred to a 25 mL round bottom flask and volatiles were removed under reduced pressure. Purification by flash column chromatography on SiO_2 (pentane/EtOAc, 3:1 v/v, $R_f = 0.4$) afforded the corresponding products **2a** as yellow solid (56.5 mg, 80% yield). **X-ray** (single-crystal) Yellow block crystals of x-ray diffraction quality was obtained by slow evaporation of saturated solution of **2a** in EtOAc/n-pentane (CCDC 2334460).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.38 (s, 1H), 7.41 – 7.27 (m, 9H), 7.16 (ddd, $J = 8.9, 4.9, 2.3$ Hz, 7H), 7.07 (d, $J = 11.9$ Hz, 1H), 5.73 – 5.56 (m, 1H), 4.32 (s, 4H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 191.2, 153.8, 151.9, 135.8, 134.6, 131.0, 129.7, 128.9, 128.1, 128.0, 127.5, 126.7, 97.1, 65.7.

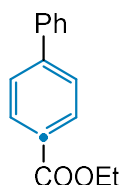


Ethyl [1,1'-biphenyl]-3-carboxylate (**4a**)

Prepared according to general procedure using 3-phenyl pyridine (29 μL , 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 μL , 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, $R_f = 0.4$) as eluent afforded **4a** as colorless oil (31.7 mg, 70% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.31 (td, *J* = 1.9, 0.5 Hz, 1H), 8.05 (ddd, *J* = 7.8, 1.7, 1.2 Hz, 1H), 7.79 (ddd, *J* = 7.8, 2.0, 1.2 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.55 – 7.44 (m, 3H), 7.42 – 7.36 (m, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.5, 141.4, 140.2, 131.4, 131.0, 128.8, 128.8, 128.3, 128.2, 127.7, 127.1, 61.0, 14.3.

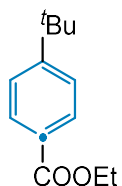


Ethyl [1,1'-biphenyl]-4-carboxylate (4b)

Prepared according to general procedure using 4-phenylpyridine (31.0 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, *R_f* = 0.4) as eluent afforded **4b** as white solid (29.2 mg, 65% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.17 – 8.07 (m, 2H), 7.70 – 7.59 (m, 4H), 7.47 (ddd, *J* = 7.8, 6.4, 1.3 Hz, 2H), 7.43 – 7.36 (m, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.5, 145.5, 140.1, 130.0, 129.3, 128.9, 128.1, 127.3, 127.0, 60.9, 14.3.

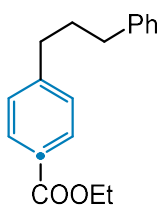


Ethyl 4-(*tert*-butyl)benzoate (4c)

Prepared according to general procedure using 4-(*tert*-butyl)pyridine (29 uL, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, *R_f* = 0.4) as eluent afforded **4c** as colorless oil (30.0 mg, 73% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.01 – 7.94 (m, 2H), 7.48 – 7.42 (m, 2H), 4.37 (q, *J* = 7.1 Hz, 2H), 1.39 (t, *J* = 7.1 Hz, 3H), 1.34 (s, 9H).

¹³C NMR (101 MHz, CDCl₃) δ 166.6, 156.4, 129.4, 127.7, 125.3, 60.7, 35.0, 31.1, 14.3.

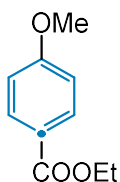


Ethyl 4-(3-phenylpropyl)benzoate (4d)

Prepared according to general procedure using 4-(3-phenylpropyl)pyridine (38 μ L, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 μ L, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, R_f = 0.4) as eluent afforded **5d** as colorless oil (31.3 mg, 58% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.03 – 7.88 (m, 2H), 7.33 – 7.14 (m, 7H), 4.35 (q, J = 7.1 Hz, 2H), 2.66 (dt, J = 20.4, 7.7 Hz, 4H), 2.04 – 1.91 (m, 2H), 1.38 (t, J = 7.1 Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.7, 147.7, 141.9, 129.6, 128.4, 128.3, 128.1, 125.8, 60.7, 35.4, 35.3, 32.6, 14.3.

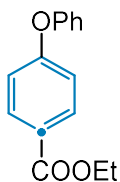


Ethyl 4-methoxybenzoate (4e)

Prepared according to general procedure using 4-methoxypyridine (20 μ L, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 μ L, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (20:1 v/v, R_f = 0.45) as eluent afforded **4e** as colorless oil (17.6 mg, 49% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.04 – 7.95 (m, 2H), 6.96 – 6.88 (m, 2H), 4.35 (q, J = 7.1 Hz, 2H), 3.86 (s, 3H), 1.38 (t, J = 7.1 Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.4, 163.2, 131.5, 123.0, 113.5, 60.6, 55.4, 14.4.

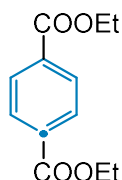


Ethyl 4-phenoxybenzoate (4f)

Prepared according to general procedure using 4-phenoxy pyridine (34.2 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 μ L, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, R_f = 0.5) as eluent afforded **4f** as colorless oil (20.2 mg, 42% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.05 – 7.97 (m, 2H), 7.43 – 7.35 (m, 2H), 7.22 – 7.15 (m, 1H), 7.09 – 7.02 (m, 2H), 7.02 – 6.95 (m, 2H), 4.36 (q, $J = 7.1$ Hz, 2H), 1.38 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.1, 161.7, 155.7, 131.6, 130.0, 124.9, 124.4, 120.0, 117.3, 60.8, 14.3.

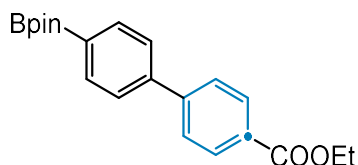


Diethyl terephthalate (4g)

Prepared according to general procedure using ethyl isonicotinate (30.2 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 μL , 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (20:1 v/v, $R_f = 0.4$) as eluent afforded **4g** as white solid (16.5 mg, 40% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.10 (s, 4H), 4.41 (q, $J = 7.1$ Hz, 4H), 1.41 (t, $J = 7.1$ Hz, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 165.9, 134.2, 129.5, 61.4, 14.3.

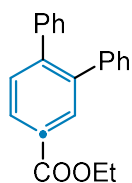


Ethyl 4'-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1'-biphenyl]-4-carboxylate (4h)

Prepared according to general procedure using 4-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)pyridine (56.2 μL , 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 μL , 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (10:1 v/v, $R_f = 0.35$) as eluent afforded **4h** as yellow solid (36.4 mg, 52% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.15 – 8.08 (m, 2H), 7.95 – 7.87 (m, 2H), 7.71 – 7.65 (m, 2H), 7.65 – 7.59 (m, 2H), 4.41 (q, $J = 7.1$ Hz, 2H), 1.42 (t, $J = 7.1$ Hz, 3H), 1.37 (s, 12H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.4, 145.3, 142.6, 135.3, 130.0, 129.5, 127.1, 126.5, 83.9, 60.9, 24.9, 14.3.

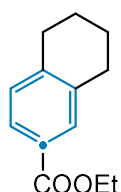


Ethyl [1,1':2',1''-terphenyl]-4'-carboxylate (4i)

Prepared according to general procedure using 3,4-diphenylpyridine (46.2 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, Rf = 0.4) as eluent afforded **4i** as yellow oil (26.4 mg, 44% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.12 (d, *J* = 1.7 Hz, 1H), 8.08 (dd, *J* = 8.0, 1.9 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.23 (dd, *J* = 4.7, 1.6 Hz, 6H), 7.19 – 7.11 (m, 4H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.4, 144.9, 140.7, 140.6, 140.6, 131.7, 130.7, 129.8, 129.7, 129.6, 128.5, 128.0, 127.1, 126.8, 61.0, 14.4.

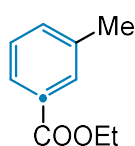


Ethyl 5,6,7,8-tetrahydronaphthalene-2-carboxylate (4j)

Prepared according to general procedure using 5,6,7,8-tetrahydroisoquinoline (26 uL, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, Rf = 0.4) as eluent afforded **4j** as yellow oil (31.1 mg, 76% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.77 – 7.70 (m, 2H), 7.13 – 7.08 (m, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 2.81 (dq, *J* = 6.7, 3.1 Hz, 4H), 1.81 (ddd, *J* = 6.7, 4.1, 2.9 Hz, 4H), 1.38 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.9, 142.7, 137.2, 130.3, 129.1, 127.6, 126.5, 60.7, 29.6, 29.3, 23.0, 22.9, 14.3.

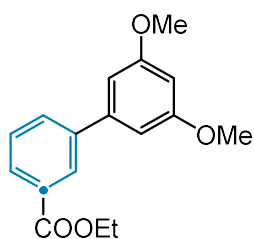


Ethyl 3-methylbenzoate (4k)

Prepared according to general procedure using 3-methylpyridine (20 uL, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, Rf = 0.4) as eluent afforded **4k** as colorless oil (11.8 mg, 36% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.91 – 7.78 (m, 2H), 7.41 – 7.28 (m, 2H), 4.37 (q, *J* = 7.1 Hz, 2H), 2.40 (d, *J* = 0.8 Hz, 3H), 1.39 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.8, 138.0, 133.5, 130.4, 130.0, 128.2, 126.6, 60.8, 21.2, 14.3.



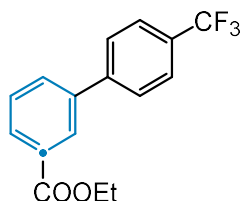
Ethyl 3',5'-dimethoxy-[1,1'-biphenyl]-3-carboxylate (**4l**)

Prepared according to general procedure using 3-(3,5-dimethoxyphenyl)pyridine (43.0 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (10:1 v/v, Rf = 0.4) as eluent afforded **4l** as colorless oil (17.3 mg, 30% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.26 (s, 1H), 8.03 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.80 – 7.71 (m, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 6.75 (d, *J* = 2.2 Hz, 2H), 6.50 (t, *J* = 2.2 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 3.86 (s, 6H), 1.42 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.5, 161.2, 142.4, 141.4, 131.5, 131.0, 128.7, 128.6, 128.2, 105.5, 99.6, 61.1, 55.5, 14.3.

HRMS (ESI): *m/z* calculated for [C₁₇H₁₈O₄] [M+Na⁺]: 309.1097, found: 309.1096.

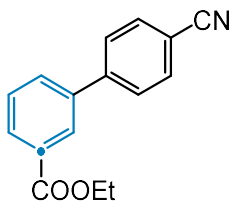


Ethyl 4'-(trifluoromethyl)-[1,1'-biphenyl]-3-carboxylate (**4m**)

Prepared according to general procedure using 3-(4-(trifluoromethyl)phenyl)pyridine (44.6 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, Rf = 0.4) as eluent afforded **4m** as colorless oil (29.3 mg, 50% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.28 (t, *J* = 1.9 Hz, 1H), 8.09 (dt, *J* = 7.8, 1.4 Hz, 1H), 7.78 (ddd, *J* = 7.7, 2.0, 1.1 Hz, 1H), 7.72 (s, 4H), 7.55 (t, *J* = 7.8 Hz, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.3, 143.7, 140.0, 131.5, 131.3, 129.8 (q, *J* = 32.7 Hz), 129.2, 129.0, 128.3, 127.5, 125.8 (q, *J* = 3.7 Hz), 124.1 (q, *J* = 271.9 Hz), 61.2, 14.3.

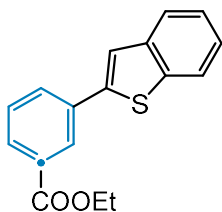


Ethyl 4'-cyano-[1,1'-biphenyl]-3-carboxylate (4n)

Prepared according to general procedure using 4-(pyridin-3-yl)benzotrile (36.0 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (5:1 v/v, $R_f = 0.3$) as eluent afforded **4n** as colorless oil (25.2 mg, 50% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.29 – 8.25 (m, 1H), 8.10 (dt, $J = 7.8, 1.4$ Hz, 1H), 7.80 – 7.69 (m, 5H), 7.56 (td, $J = 7.8, 0.5$ Hz, 1H), 4.42 (q, $J = 7.1$ Hz, 2H), 1.42 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.1, 144.6, 139.4, 132.7, 131.4, 131.4, 129.6, 129.2, 128.3, 127.8, 118.7, 111.4, 61.3, 14.3.

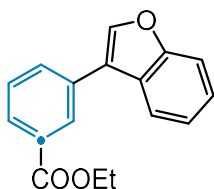


Ethyl 3-(benzo[b]thiophen-2-yl)benzoate (4o)

Prepared according to general procedure using 3-(benzo[b]thiophen-2-yl)pyridine (42.2 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (20:1 v/v, $R_f = 0.3$) as eluent afforded **4o** as white solid (25.2 mg, 45% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.40 (s, 1H), 8.02 (dd, $J = 7.9, 1.3$ Hz, 1H), 7.91 – 7.83 (m, 2H), 7.82 – 7.77 (m, 1H), 7.63 (s, 1H), 7.50 (t, $J = 7.8$ Hz, 1H), 7.40 – 7.31 (m, 2H), 4.44 (q, $J = 7.1$ Hz, 2H), 1.44 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.2, 143.0, 140.5, 139.6, 134.6, 131.3, 130.6, 129.1, 129.0, 127.4, 124.6, 124.6, 123.7, 122.3, 120.2, 61.2, 14.3.



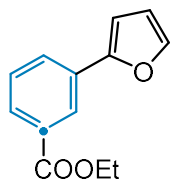
Ethyl 3-(benzofuran-3-yl)benzoate (4p)

Prepared according to general procedure using 3-(benzofuran-3-yl)pyridine (39.0 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (20:1 v/v, Rf = 0.4) as eluent afforded **4p** as colorless oil (23.7 mg, 45% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.34 (td, *J* = 1.8, 0.5 Hz, 1H), 8.05 (dt, *J* = 7.9, 1.4 Hz, 1H), 7.88 – 7.82 (m, 3H), 7.60 – 7.52 (m, 2H), 7.42 – 7.32 (m, 2H), 4.43 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.4, 155.8, 141.7, 132.4, 131.6, 131.3, 129.0, 128.5, 126.2, 124.7, 123.2, 121.5, 120.2, 111.8, 61.1, 14.3.

HRMS (ESI): m/z calculated for [C₁₇H₁₄O₃] [M+Na⁺]: 289.0835, found: 289.0833.



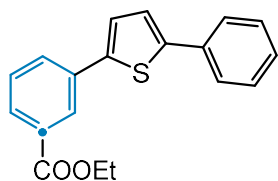
Ethyl 3-(furan-2-yl)benzoate (**4q**)

Prepared according to general procedure using 3-(furan-2-yl)pyridine (29.0 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (20:1 v/v, Rf = 0.4) as eluent afforded **4q** as colorless oil (17.1 mg, 40% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.33 (t, *J* = 1.8 Hz, 1H), 7.93 (dt, *J* = 7.8, 1.5 Hz, 1H), 7.85 (dt, *J* = 7.8, 1.5 Hz, 1H), 7.50 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 6.74 (dd, *J* = 3.4, 0.8 Hz, 1H), 6.50 (dd, *J* = 3.4, 1.8 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.4, 153.0, 142.5, 132.9, 131.1, 128.7, 128.2, 127.8, 124.9, 111.8, 105.8, 61.1, 14.3.

HRMS (ESI): m/z calculated for [C₁₃H₁₂O₃] [M+Na⁺]: 239.0679, found: 239.0677.



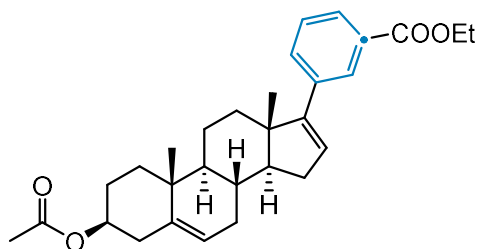
Ethyl 3-(5-phenylthiophen-2-yl)benzoate (**4r**)

Prepared according to general procedure using 3-(5-phenylthiophen-2-yl)pyridine (47.4 mg, 0.2 mmol), ethyl 2-(diethoxyphosphoryl)acetate (80 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (20:1 v/v, Rf = 0.4) as eluent afforded **4r** as colorless oil (26.3 mg, 43% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.34 – 8.28 (m, 1H), 7.96 (dt, *J* = 7.9, 1.4 Hz, 1H), 7.80 (ddd, *J* = 7.8, 2.0, 1.1 Hz, 1H), 7.67 – 7.62 (m, 2H), 7.46 (td, *J* = 7.8, 0.5 Hz, 1H), 7.43 – 7.35 (m, 3H), 7.33 – 7.28 (m, 2H), 4.43 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.3, 144.3, 142.3, 134.6, 134.1, 131.2, 129.7, 128.9, 128.3, 127.7, 126.5, 125.7, 124.7, 124.1, 61.2, 14.3.

HRMS (ESI): *m/z* calculated for [C₁₉H₁₆O₂S] [M+Na⁺]: 331.0763, found: 331.0762.

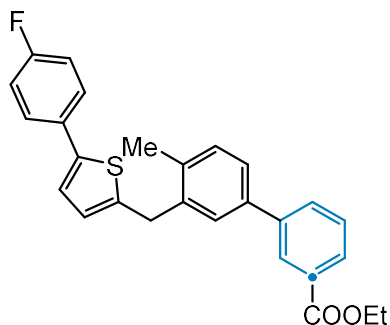


Ethyl 3-((3S,8R,9S,10R,13S,14S)-3-acetoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15-dodecahydro-1H-cyclopenta[a]phenanthren-17-yl)benzoate (4s)

Prepared according to general procedure using abiraterone acetate (78.2 mg, 0.2 mmol), dimethyl (2-oxopropyl)phosphonate (55 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (10:1 v/v, R_f = 0.3) as eluent afforded **4s** as white solid (51.0 mg, 55% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.16 (d, *J* = 15.8 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.23 (d, *J* = 7.2 Hz, 1H), 7.12 (t, *J* = 7.6 Hz, 1H), 6.29 (d, *J* = 15.8 Hz, 1H), 5.42 (d, *J* = 4.9 Hz, 1H), 4.62 (ddd, *J* = 11.5, 8.5, 3.5 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 2.74 (dd, *J* = 14.7, 6.4 Hz, 1H), 2.56 – 2.47 (m, 2H), 2.40 – 2.32 (m, 2H), 2.13 – 2.07 (m, 1H), 2.04 (s, 3H), 1.92 – 1.86 (m, 2H), 1.81 – 1.62 (m, 7H), 1.34 (t, *J* = 7.1 Hz, 3H), 1.18 – 1.11 (m, 2H), 1.10 (s, 3H), 1.06 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 170.5, 167.1, 152.7, 143.8, 142.6, 140.0, 130.5, 126.6, 126.4, 124.4, 122.1, 119.0, 73.8, 60.4, 57.0, 50.0, 47.0, 38.1, 37.1, 36.8, 36.7, 32.3, 31.6, 30.7, 27.7, 21.4, 21.0, 19.3, 17.7, 14.3.



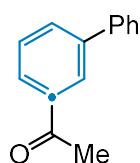
Ethyl 3'-((5-(4-fluorophenyl)thiophen-2-yl)methyl)-4'-methyl-[1,1'-biphenyl]-3-carboxylate (4t)

Prepared according to general procedure using 3-(3-((5-(4-fluorophenyl)thiophen-2-yl)methyl)-4-methylphenyl)pyridine (71.8 mg, 0.2 mmol), dimethyl (2-oxopropyl)phosphonate (55 uL, 2.0 equiv.)

were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (20:1 v/v, Rf = 0.3) as eluent afforded **4t** as colorless oil (30.1 mg, 42% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.27 (t, *J* = 1.8 Hz, 1H), 8.00 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.77 (ddd, *J* = 7.7, 1.9, 1.2 Hz, 1H), 7.52 – 7.43 (m, 5H), 7.28 (d, *J* = 7.9 Hz, 1H), 7.06 – 6.97 (m, 3H), 6.73 – 6.68 (m, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 4.21 (s, 2H), 2.38 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.6, 162.1 (d, *J* = 246.7 Hz), 143.2, 141.6, 141.2, 138.7, 138.1, 136.1, 131.3, 131.1, 131.0, 130.8 (d, *J* = 3.4 Hz), 128.8, 128.3, 128.1, 128.0, 127.1 (d, *J* = 8.0 Hz), 126.0, 125.7, 122.7, 115.7 (d, *J* = 21.8 Hz), 61.1, 34.3, 19.2, 14.3.

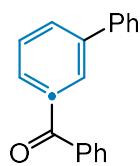


1-([1,1'-Biphenyl]-3-yl)ethan-1-one (**5a**)

Prepared according to general procedure using 3-phenylpyridine (29 uL, 0.2 mmol), dimethyl (2-oxopropyl)phosphonate (55 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, Rf = 0.4) as eluent afforded **5a** as yellow oil (17.4 mg, 44% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.19 (td, *J* = 1.9, 0.5 Hz, 1H), 7.94 (ddd, *J* = 7.8, 1.8, 1.1 Hz, 1H), 7.80 (ddd, *J* = 7.7, 1.9, 1.1 Hz, 1H), 7.65 – 7.59 (m, 2H), 7.54 (td, *J* = 7.7, 0.6 Hz, 1H), 7.51 – 7.43 (m, 2H), 7.42 – 7.36 (m, 1H), 2.66 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 198.1, 141.7, 140.2, 137.6, 131.7, 129.0, 128.9, 127.8, 127.2, 127.2, 127.0, 26.7.

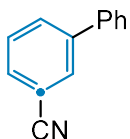


[1,1'-Biphenyl]-3-yl(phenyl)methanone (**5b**)

Prepared according to general procedure using 3-phenylpyridine (29 uL, 0.2 mmol), diethyl (2-oxo-2-phenylethyl)phosphonate (87 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, Rf = 0.4) as eluent afforded **5b** as colorless oil (20.8 mg, 40% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.06 – 8.01 (m, 1H), 7.90 – 7.84 (m, 2H), 7.82 (ddd, *J* = 7.7, 1.9, 1.2 Hz, 1H), 7.77 (dt, *J* = 7.8, 1.4 Hz, 1H), 7.61 (ddt, *J* = 8.2, 6.7, 1.4 Hz, 3H), 7.56 (t, *J* = 7.7 Hz, 1H), 7.53 – 7.44 (m, 4H), 7.41 – 7.36 (m, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 196.7, 141.4, 140.2, 138.2, 137.6, 132.5, 131.0, 130.1, 128.9, 128.7, 128.6, 128.3, 127.8, 127.2.

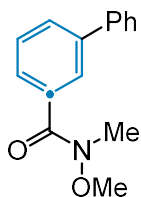


[1,1'-Biphenyl]-3-carbonitrile (**5c**)

Prepared according to general procedure using 3-phenylpyridine (29 uL, 0.2 mmol), diethyl (cyanomethyl)phosphonate (65 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, R_f = 0.4) as eluent afforded **5c** as yellow oil (22.1 mg, 62% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.89 – 7.84 (m, 1H), 7.82 (ddd, *J* = 7.9, 1.9, 1.3 Hz, 1H), 7.63 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.59 – 7.52 (m, 3H), 7.48 (ddd, *J* = 8.2, 7.0, 1.0 Hz, 2H), 7.45 – 7.39 (m, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 142.4, 138.9, 131.5, 130.7, 130.7, 129.6, 129.1, 128.4, 127.1, 118.8, 112.9.

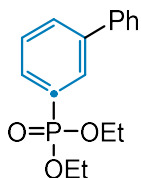


N-Methoxy-*N*-methyl-[1,1'-biphenyl]-3-carboxamide (**5d**)

Prepared according to general procedure using 3-phenylpyridine (29 uL, 0.2 mmol), diethyl (2-(methoxy(methyl)amino)-2-oxoethyl)phosphonate (82 uL, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (2:1 v/v, R_f = 0.4) as eluent afforded **5d** as yellow oil (26.8 mg, 56% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.90 (t, *J* = 1.8 Hz, 1H), 7.69 (ddd, *J* = 7.7, 1.9, 1.2 Hz, 1H), 7.66 – 7.58 (m, 3H), 7.51 – 7.43 (m, 3H), 7.39 – 7.33 (m, 1H), 3.59 (s, 3H), 3.39 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 169.9, 141.0, 140.4, 134.7, 129.2, 128.8, 128.5, 127.6, 127.1, 126.9, 126.9, 61.1, 33.8.



Diethyl [1,1'-biphenyl]-3-ylphosphonate (**5e**)

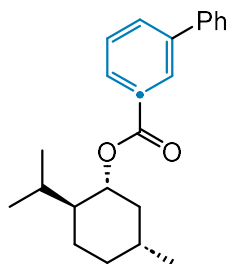
Prepared according to general procedure using 3-phenylpyridine (29 uL, 0.2 mmol), tetraethyl methylenebis(phosphonate) (99 uL, 2.0 equiv.) were used. Purification by column chromatography

using pre-basified silica with EtOAc ($R_f = 0.4$) as eluent afforded **5e** as yellow oil (22.0 mg, 38% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.04 (dt, $J = 14.2, 1.8$ Hz, 1H), 7.83 – 7.75 (m, 2H), 7.63 – 7.58 (m, 2H), 7.54 (td, $J = 7.7, 4.4$ Hz, 1H), 7.49 – 7.42 (m, 2H), 7.40 – 7.36 (m, 1H), 4.25 – 4.06 (m, 4H), 1.34 (t, $J = 7.1$ Hz, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 141.5 (d, $J = 15.0$ Hz), 140.0, 140.0, 131.0 (d, $J = 3.2$ Hz), 130.5 (d, $J = 5.9$ Hz), 130.4 (d, $J = 6.8$ Hz), 128.9 (d, $J = 15.7$ Hz), 128.9, 127.8, 127.2, 62.2, 62.1, 16.4, 16.3.

$^{31}\text{P NMR}$ (162 MHz, CDCl_3) δ 18.71.



(1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl [1,1'-biphenyl]-3-carboxylate (5f)

Prepared according to general procedure using 3-phenylpyridine (29 μL , 0.2 mmol), (1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 2-(diethoxyphosphoryl)acetate (133.6 mg, 2.0 equiv.) were used. Purification by column chromatography using pre-basified silica with pentane/EtOAc (50:1 v/v, $R_f = 0.4$) as eluent afforded **5f** as colorless oil (31.2 mg, 47% yield).

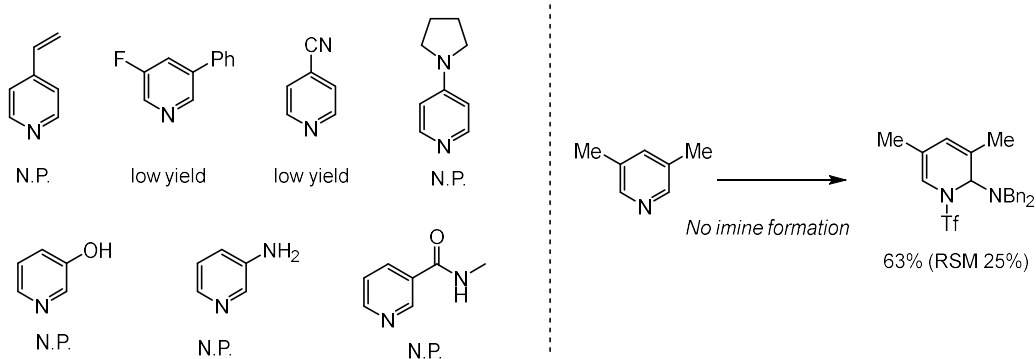
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.28 (t, $J = 1.8$ Hz, 1H), 8.04 (dt, $J = 7.8, 1.4$ Hz, 1H), 7.78 (ddd, $J = 7.7, 2.0, 1.2$ Hz, 1H), 7.66 – 7.61 (m, 2H), 7.54 – 7.45 (m, 3H), 7.42 – 7.37 (m, 1H), 4.99 (td, $J = 10.9, 4.4$ Hz, 1H), 2.15 (dtd, $J = 12.0, 4.0, 1.7$ Hz, 1H), 1.98 (ddt, $J = 14.0, 7.0, 3.5$ Hz, 1H), 1.78 – 1.71 (m, 2H), 1.62 – 1.55 (m, 2H), 1.19 – 1.08 (m, 2H), 0.94 (dd, $J = 6.8, 5.5$ Hz, 7H), 0.82 (d, $J = 6.9$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.0, 141.5, 140.3, 131.4, 131.4, 128.9, 128.8, 128.3, 128.2, 127.7, 127.2, 75.0, 47.3, 41.0, 34.3, 31.5, 26.5, 23.7, 22.0, 20.8, 16.6.

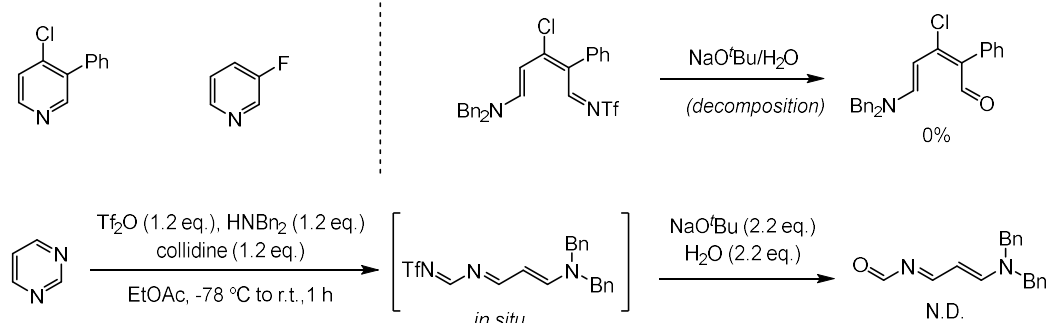
4. Limitations

4.1 limitation of pyridines

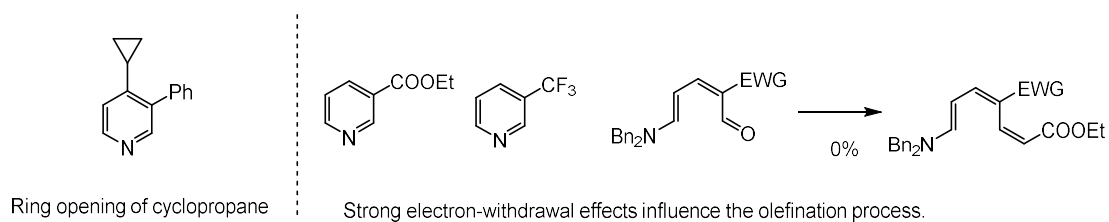
i) No imine or low-yielding imine formation



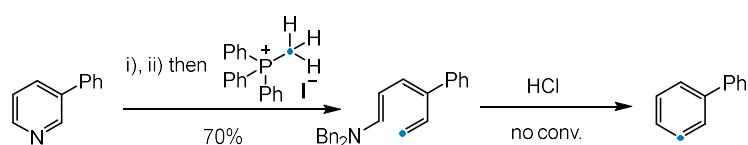
ii) Problematic hydrolysis step



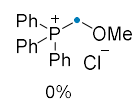
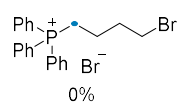
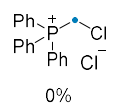
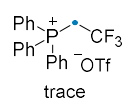
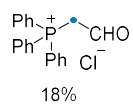
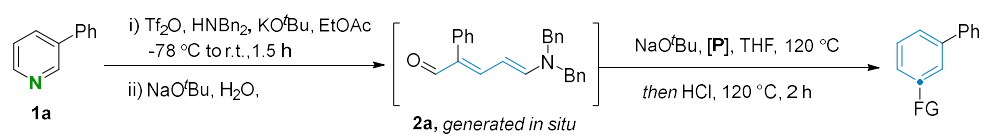
iii) Low yielding alkene formation during olefination step



iv) Problematic ring closure step



4.2 limitation of phosphine reagents



5. X-Ray analysis

X-Ray diffraction: Data sets for compound **2a** were collected with a Bruker D8 Venture Photon III Diffractometer. Programs used: data collection: *APEX4* Version 2021.4-0¹ (Bruker AXS Inc., **2021**); cell refinement: *SAINT* Version 8.40B (Bruker AXS Inc., **2021**); data reduction: *SAINT* Version 8.40B (Bruker AXS Inc., **2021**); absorption correction, *SADABS* Version 2016/2 (Bruker AXS Inc., **2021**); structure solution *SHELXT*-Version 2018-3² (Sheldrick, G. M. *Acta Cryst.*, **2015**, *A71*, 3-8); structure refinement *SHELXL*-Version 2018-3³ (Sheldrick, G. M. *Acta Cryst.*, **2015**, *C71* (1), 3-8) and graphics, *XP*⁴ (Version 5.1, Bruker AXS Inc., Madison, Wisconsin, USA, **1998**). *R*-values are given for observed reflections, and *wR*² values are given for all reflections.

X-ray crystal structure analysis of 2a: A orange-yellow, block-like specimen of C₂₅H₂₃NO, approximate dimensions 0.074 mm x 0.090 mm x 0.110 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a single crystal diffractometer Bruker D8 Venture Photon III system equipped with a micro focus tube Cu ImS (CuK α , λ = 1.54178 Å) and a MX mirror monochromator. A total of 1432 frames were collected. The total exposure time was 22.40 hours. The frames were integrated with the Bruker SAINT software package using a wide-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 29807 reflections to a maximum θ angle of 66.68° (0.84 Å resolution), of which 3305 were independent (average redundancy 9.019, completeness = 99.4%, *R*_{int} = 9.09%, *R*_{sig} = 3.84%) and 2617 (79.18%) were greater than 2 σ (*F*²). The final cell constants of *a* = 16.5300(3) Å, *b* = 5.94310(10) Å, *c* = 20.4998(4) Å, β = 110.4490(10)°, volume = 1886.98(6) Å³, are based upon the refinement of the XYZ-centroids of 8534 reflections above 20 σ (*I*) with 5.948° < 2 θ < 132.7°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.918. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9390 and 0.9580. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group *P*₂₁/*n*, with *Z* = 4 for the formula unit, C₂₅H₂₃NO. The final anisotropic full-matrix least-squares refinement on *F*² with 244 variables converged at *R*1 = 4.18%, for the observed data and *wR*2 = 10.30% for all data. The goodness-of-fit was 1.049. The largest peak in the

final difference electron density synthesis was $0.247 \text{ e}^-/\text{\AA}^3$ and the largest hole was $-0.181 \text{ e}^-/\text{\AA}^3$ with an RMS deviation of $0.039 \text{ e}^-/\text{\AA}^3$. On the basis of the final model, the calculated density was 1.244 g/cm^3 and $F(000)$, 752 e^- . CCDC Nr.: 2334460.

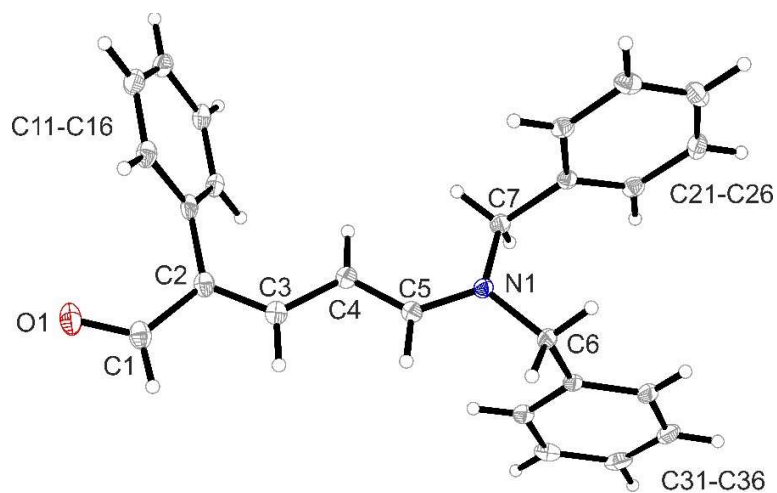


Figure S1. Crystal structure of compound **2a**. Thermal ellipsoids are shown at 30% probability.

6. DFT calculation

Computational Details

All geometry optimizations of intermediates and transition states were achieved using spin-unrestricted UB3LYP⁵-D3⁶/def2-SVP⁷ method, in tetrahydrofuran solvent using the CPCM solvent model⁸ with “opt=noeigen” and “guess=mix” keywords as implemented in Gaussian16⁹. Frequency calculations were also conducted at the same level of theory to obtain vibrational frequencies to determine the identity of stationary points as intermediates (no imaginary frequencies) or transition states (only one imaginary frequency), as well as obtaining the thermochemistry: enthalpy (ΔH) and free energy (ΔG) at the temperature of 298 K. Single point energy calculations were done using the following methods:

UB3LYP-D3/def2TZVPP-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)

UB3LYP-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)

UPBEPBE-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)

UM06/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF).

Extensive conformational analysis was done for all key transition states and stationary points and the minimum energy structures were chosen for the minimum energy profiles. All structural figures were generated with CYLview.¹⁰ Distances in structural figures are shown in Å and energies are in kcal/mol.

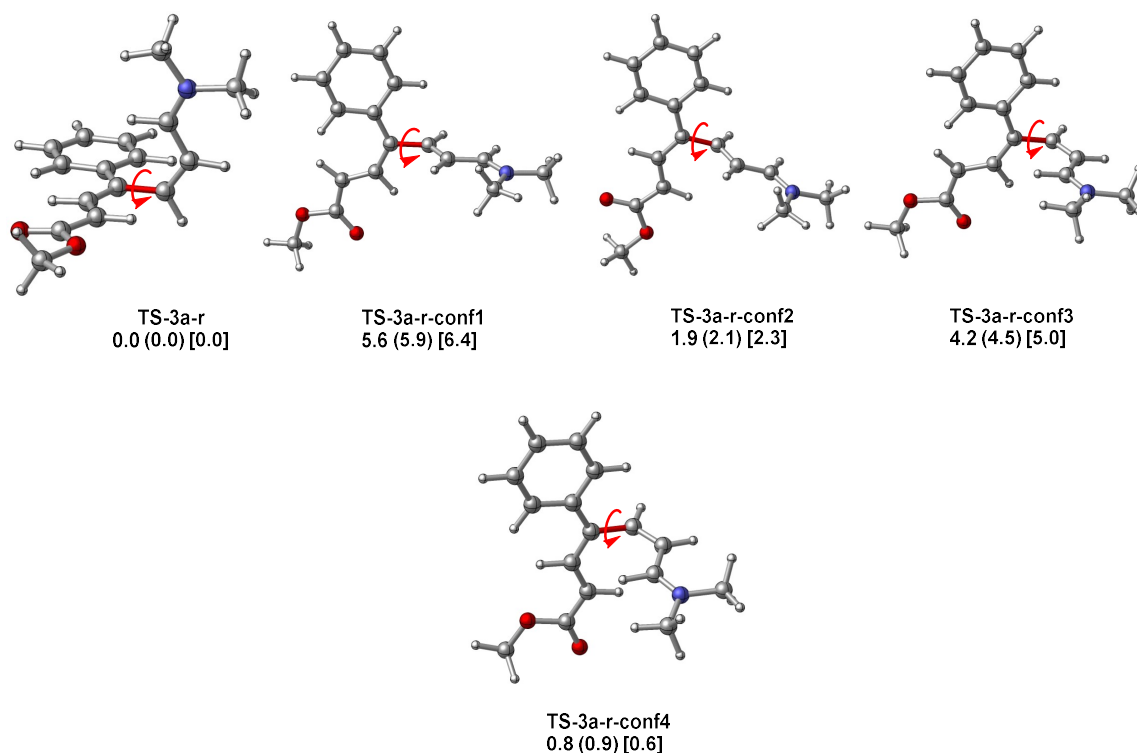


Figure S2. Different conformations for the C_7 - C_8 rotation transition state for substrate **3a** calculated at the theoretical level: UB3LYP-d3/def2-svp-CPCM(THF). Calculated energies, enthalpy (parentheses) and free Gibbs energies [brackets] are given in kcal mol⁻¹.

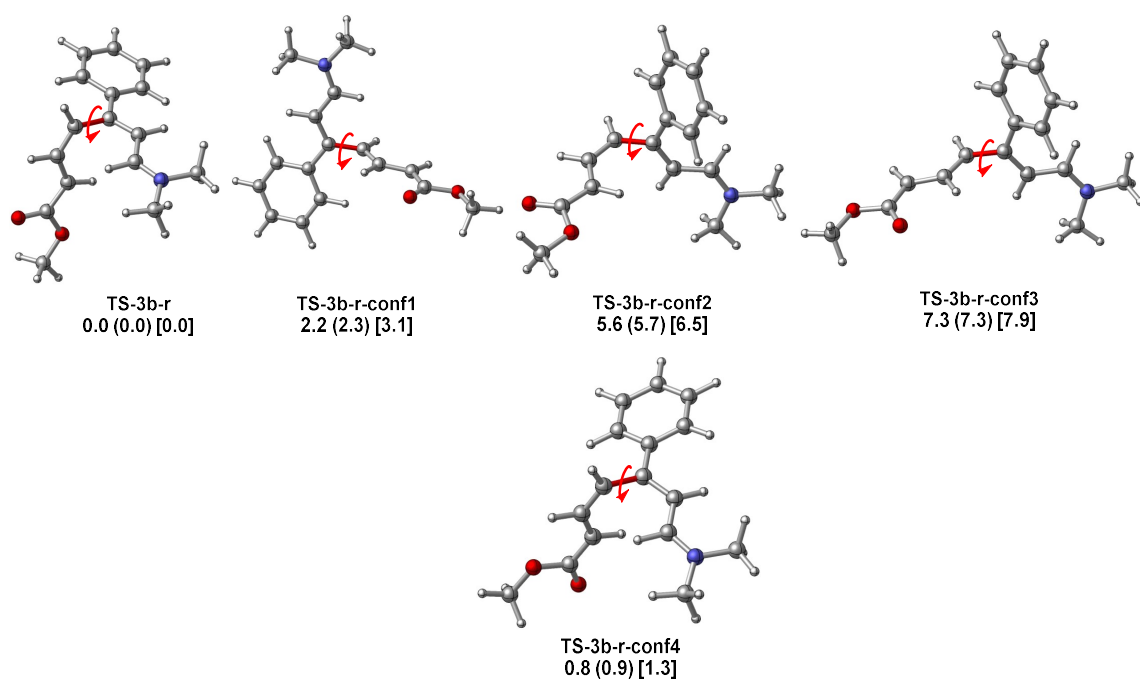


Figure S3. Different conformations for the C_7 - C_8 rotation transition state for substrate **3b** calculated at the theoretical level: UB3LYP-d3/def2-svp-CPCM(THF). Calculated energies, enthalpy (parentheses) and free Gibbs energies [brackets] are given in kcal mol⁻¹.

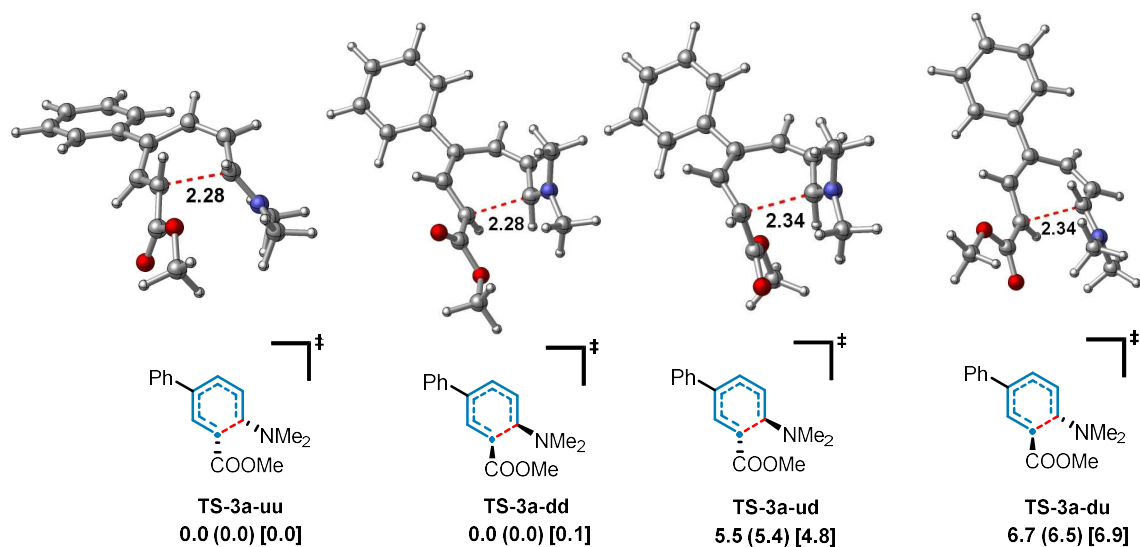


Figure S4. Different conformations for the electrocyclization transition state for substrate **3a** calculated at the theoretical level: UB3LYP-d3/def2-svp-CPCM(THF). Calculated energies, enthalpy (parentheses) and free Gibbs energies [brackets] are given in kcal mol⁻¹.

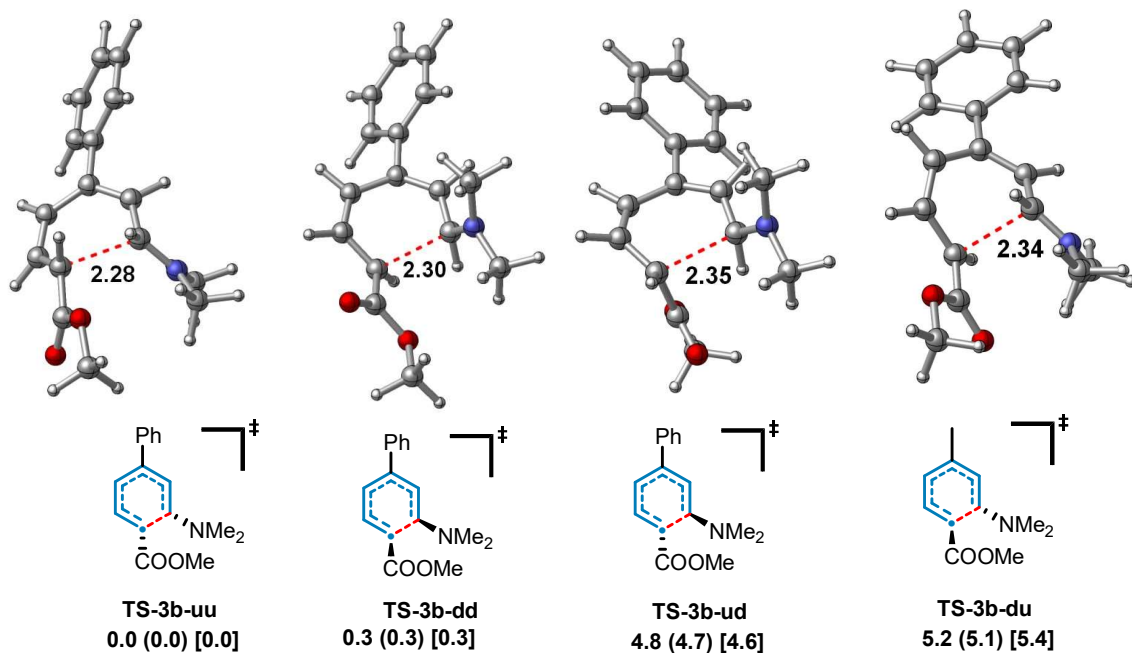


Figure S5. Different conformations for the electrocyclicization transition state for substrate **3b** calculated at the theoretical level: UB3LYP-d3/def2-svp-CPCM(THF). Calculated energies, enthalpy (parentheses) and free Gibbs energies [brackets] are given in kcal mol⁻¹.

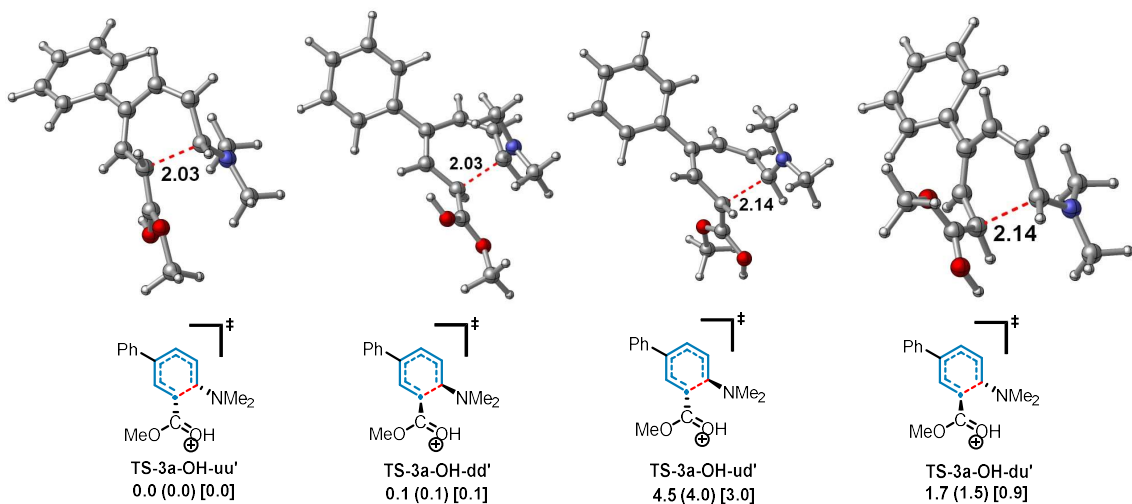


Figure S6. Different conformations for the electrocyclicization transition state for the protonated substrate **3a-OH** (without chloride as counter-ion) calculated at the theoretical level: UB3LYP-d3/def2-svp-CPCM(THF). Calculated energies, enthalpy (parentheses) and free Gibbs energies [brackets] are given in kcal mol⁻¹.

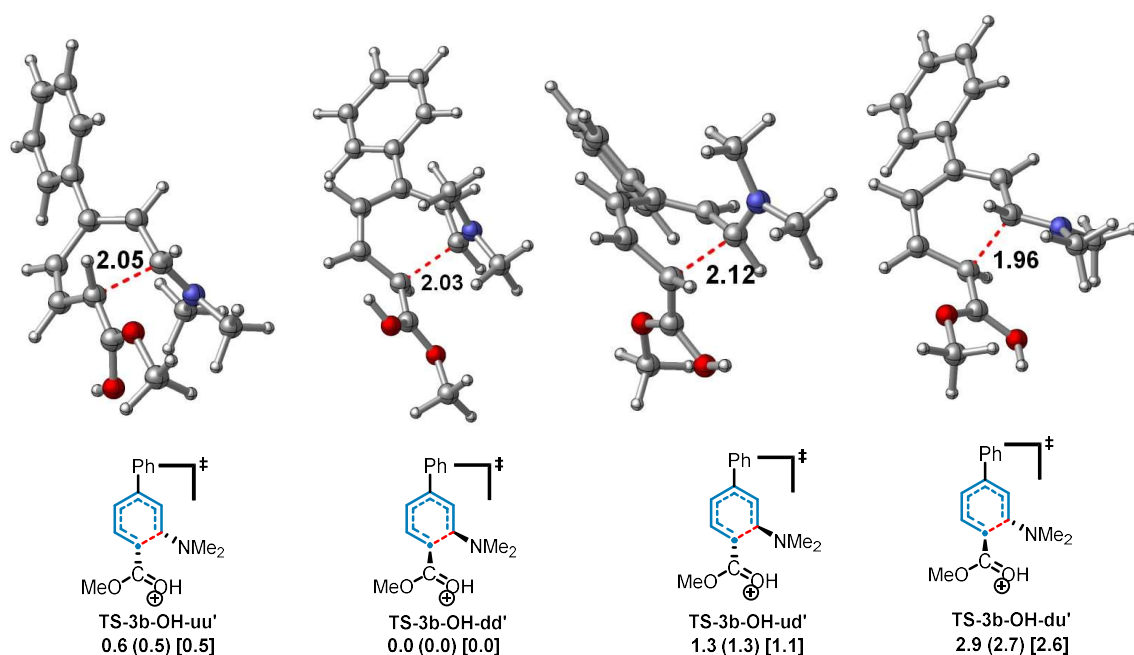
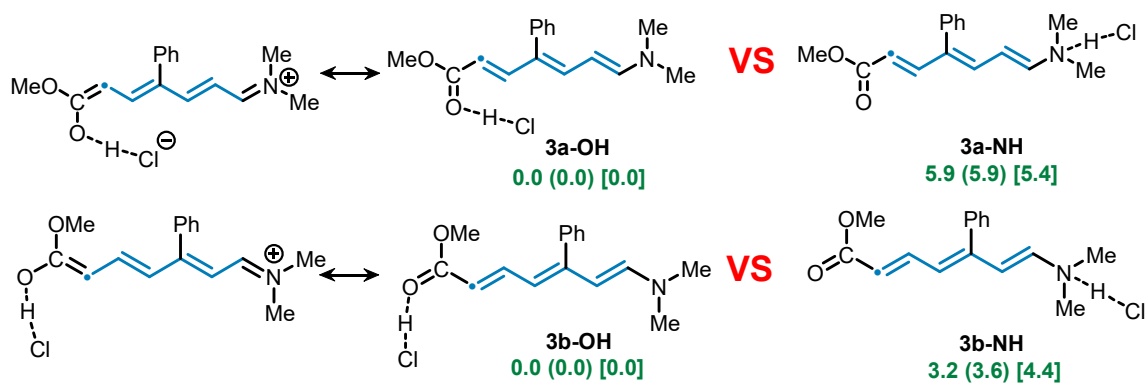


Figure S7. Different conformations for the electrocyclicization transition state for the protonated substrate **3b-OH** (without chloride as counter-ion) calculated at the theoretical level: UB3LYP-d3/def2-svp-CPCM(THF). Calculated energies, enthalpy (parentheses) and free Gibbs energies [brackets] are given in kcal mol⁻¹.

UB3LYP-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)
 ΔE (ΔH) [ΔG] in kcal/mol



Stabilization of 3a-OH and 3b-OH over 3a-NH and 3b-NH due to extended delocalization

Figure S8. Energy preferences for protonation at the carbonyl oxygen over the nitrogen due to extended delocalization calculated at the theoretical level: UB3LYP-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-d3/def2-svp-CPCM(THF). Calculated energies, enthalpy (parentheses) and free Gibbs energies [brackets] are given in kcal mol⁻¹.

- Under acidic conditions, Carbonyl oxygen gets protonated rather than N.

- Thermodynamically, protonation of carbonyl O is favored over N.
- If carbonyl oxygen gets protonated, the positive charge can delocalize, and this also helps in lowering the barrier of rotation whereas that is not possible if N gets protonated.

UB3LYP-D3/def2svp-CPCM(THF)

UB3LYP-D3/def2TZVPP-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)

UB3LYP-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)

UPBEPBE-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)

UM06/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)

ΔE (ΔH) [ΔG] in kcal/mol

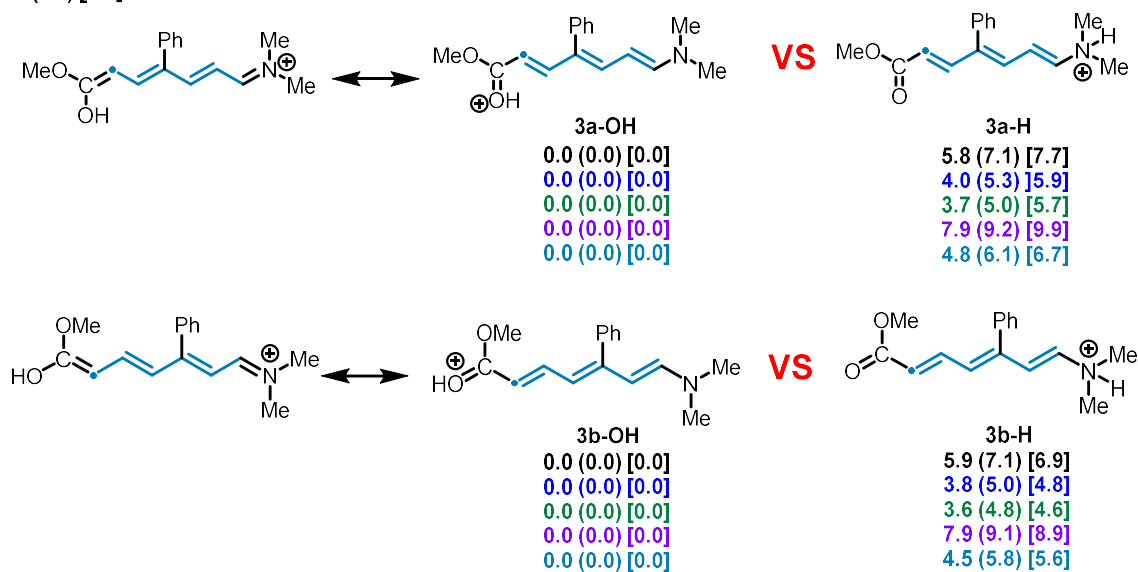


Figure S9. Energy preferences for protonation at the carbonyl oxygen over the nitrogen due to extended delocalization calculated at different methods without the chloride as counter-ion. Calculated energies, enthalpy (parentheses) and free Gibbs energies [brackets] are given in kcal mol⁻¹.

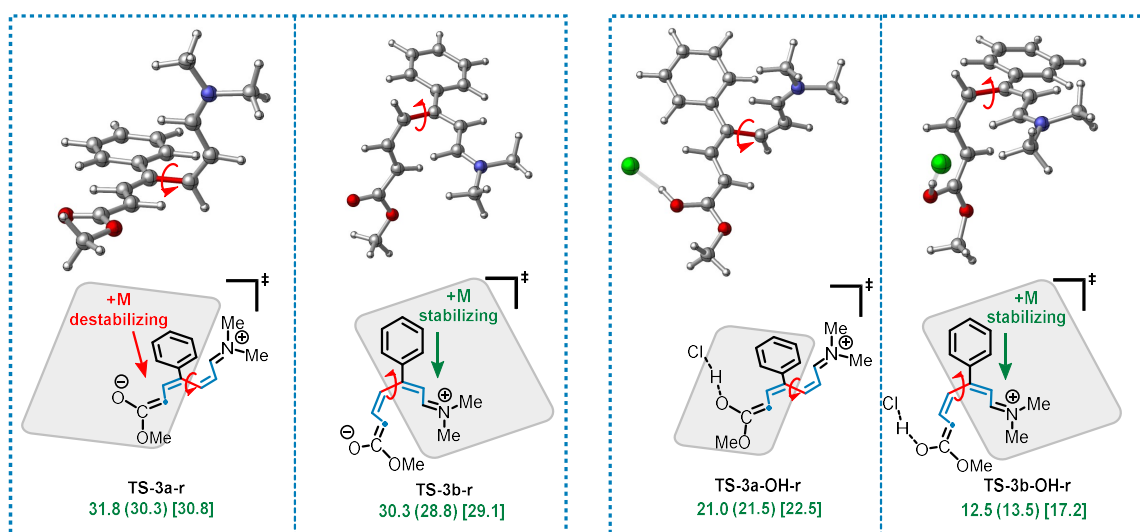


Figure S10. Key C_7 - C_8 rotation transition states for substrates **3a** and **3b** under basic (left) and acidic (right) conditions, highlighting the effect of protonation in lowering the rotation barrier calculated at the theoretical level: UB3LYP-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-d3/def2-svp-CPCM(THF). Calculated energies, enthalpy (parentheses) and free Gibbs energies [brackets] are given in kcal mol⁻¹.

Under basic conditions, the barrier for double bond rotation for the 3-substituted substrate (**3a**) is around 1.7 kcal higher as compared to the 4-substituted substrate (**3b**) consistent with experiments. Under acidic conditions that barrier becomes much lower (below 20 kcal) presumably because of the resonance structure shown above in which the double bond in question has reduced π -bond character.

TS-3b-r has lower barrier because in that TS, the phenyl ring is in the same plane as the NMe₂ group thus stabilizing the positive charge on N via +M effect. The Opposite is true for **TS-3a-r** where phenyl ring destabilizes the negative charge on O.

UB3LYP-D3/def2svp-CPCM(THF)
 UB3LYP-D3/def2TZVPP-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)
 UB3LYP-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)
 UPBEPBE-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)
 UMO6/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)
 ΔE (ΔH) [ΔG] in kcal/mol

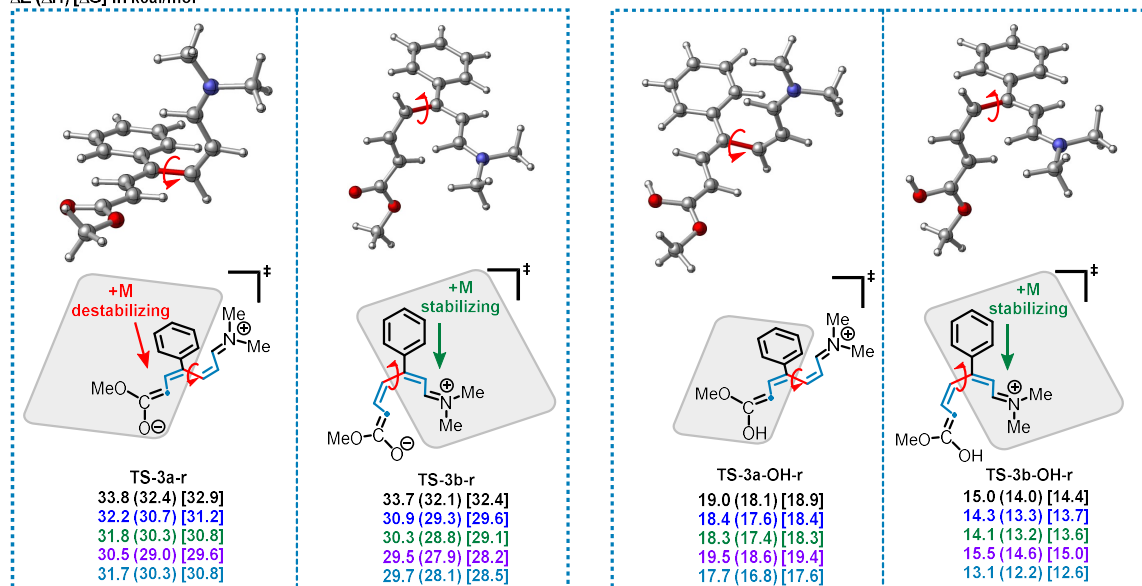


Figure S11. Key C_7 - C_8 rotation transition states for substrates **3a** and **3b** under basic (left) and acidic (right) conditions without the chloride as counter-ion, highlighting the effect of protonation in lowering the rotation barrier calculated at different methods. Calculated energies, enthalpy (parentheses) and free Gibbs energies [brackets] are given in kcal mol⁻¹.

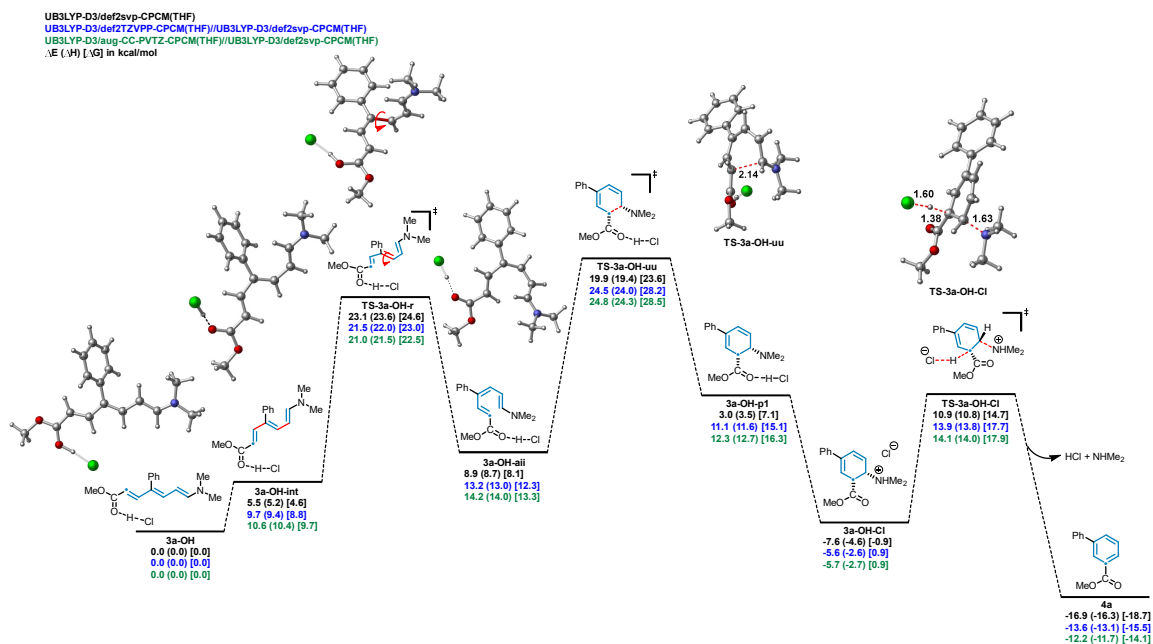


Figure S12. Full minimum energy pathway for substrate **3a** under acidic conditions calculated at different methods.

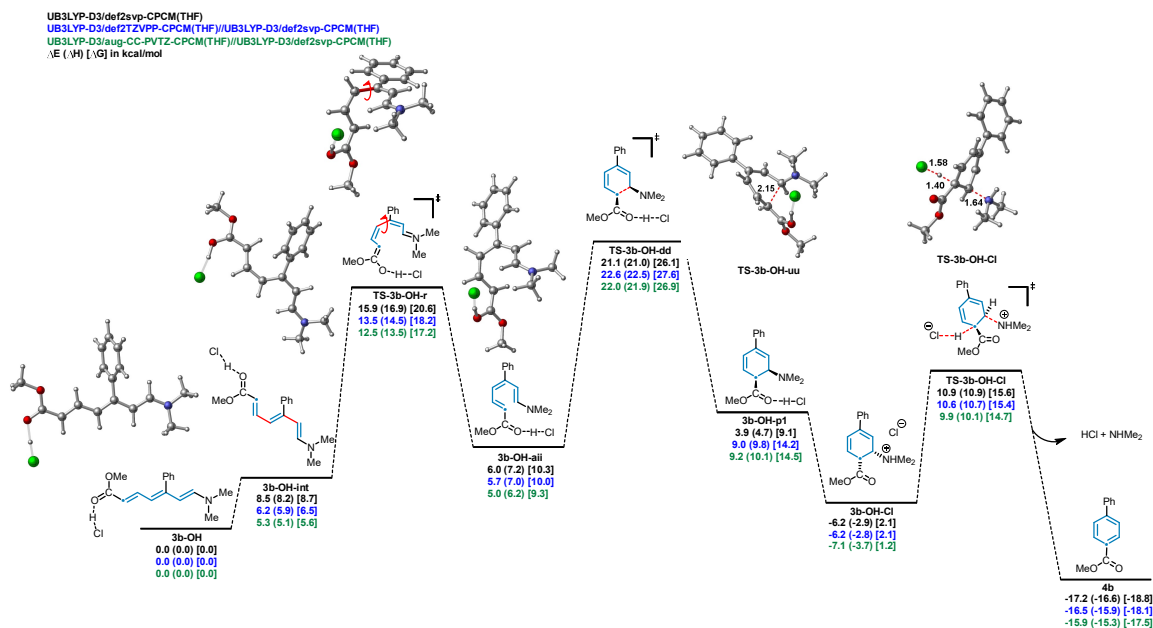


Figure S13. Full minimum energy pathway for substrate **3b** under acidic conditions calculated at different methods.

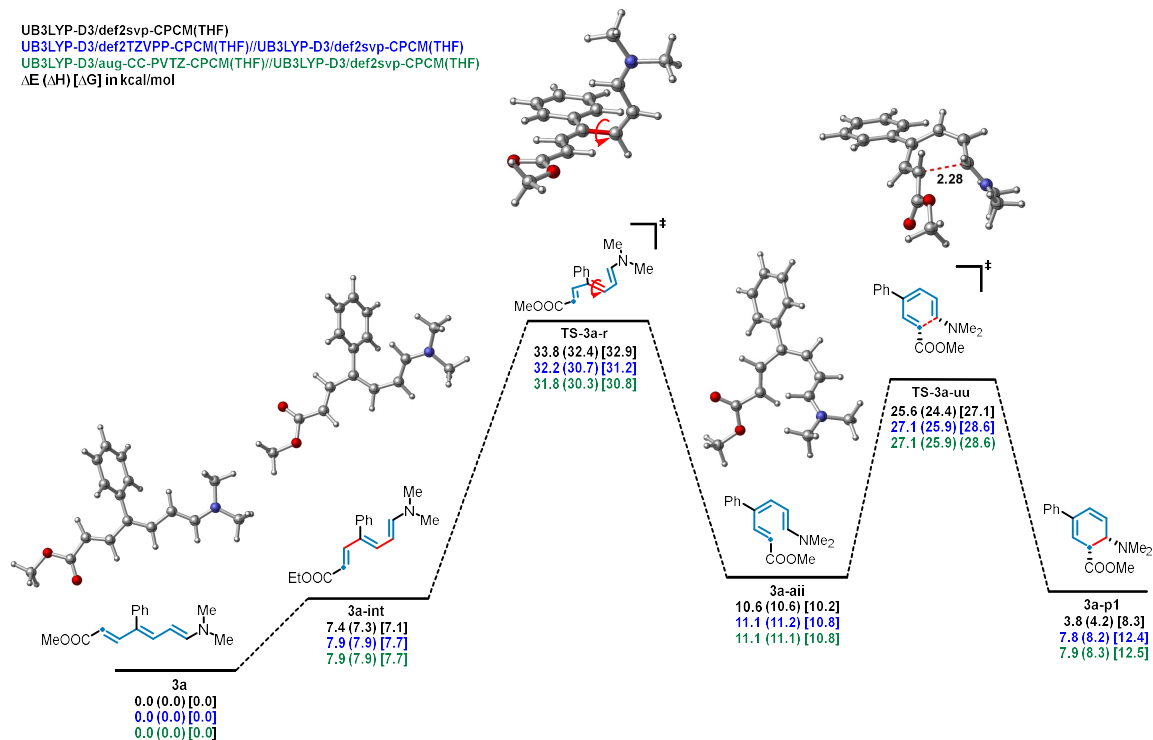


Figure S14. Minimum energy pathway for substrate **3a** under basic conditions till electrocyclization step calculated at different methods.

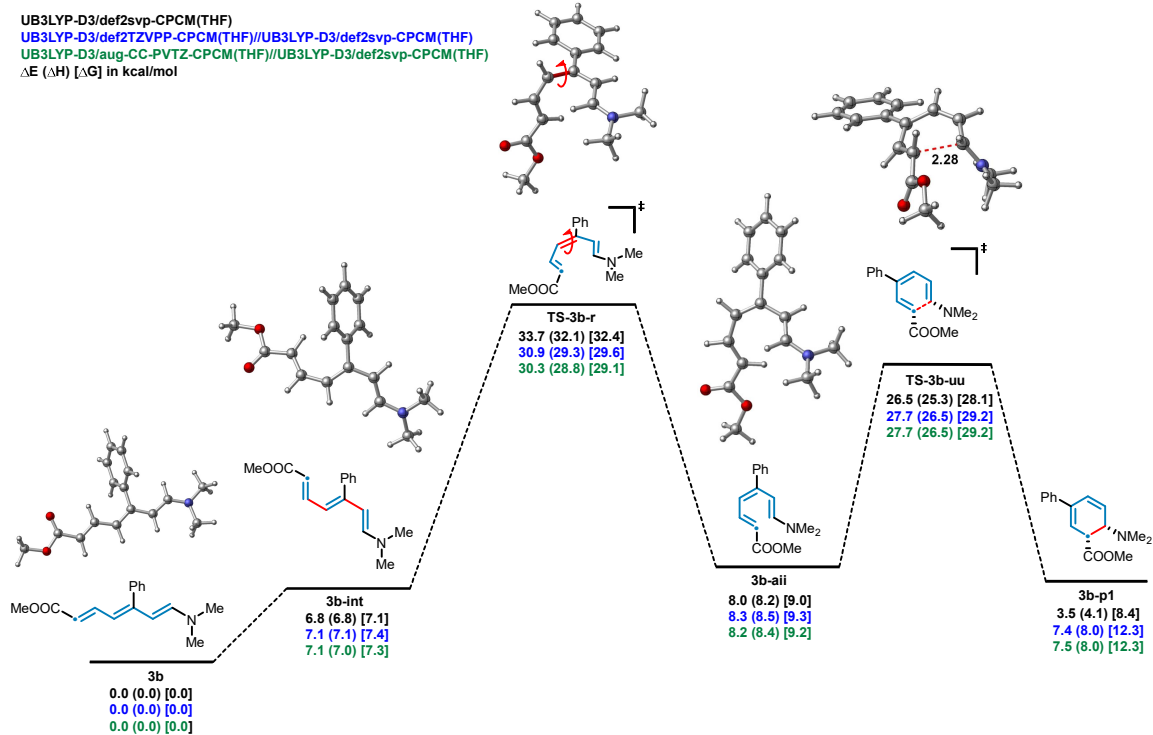


Figure S15. Minimum energy pathway for substrate **3b** under basic conditions till electrocyclization step calculated at different methods.

UB3LYP-D3/def2svp-CPCM(THF)
 UB3LYP-D3/def2TZVP-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)
 UB3LYP-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)
 UPBEPBE-D3/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)
 UM06/aug-CC-PVTZ-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF)
 ΔE (ΔH) [ΔG] in kcal/mol

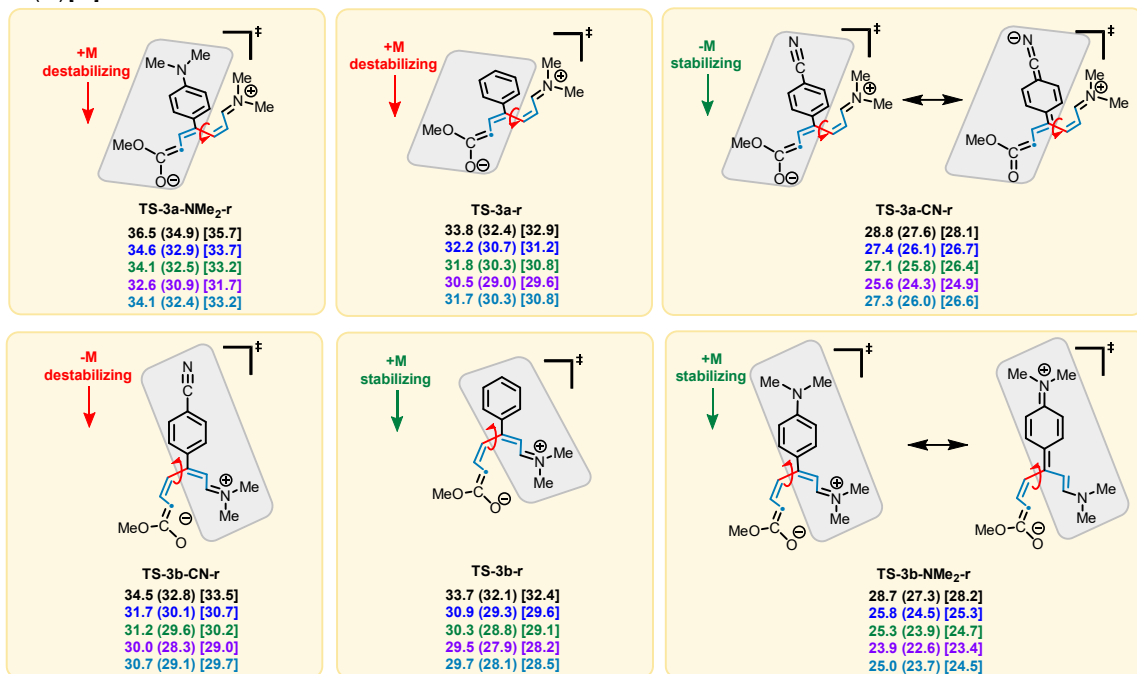


Figure S16. Probing the effect of electron donating and withdrawing groups in the key C_γ - C_δ rotation transition states for substrates **3a** and **3b** under basic conditions.

Increasing +M effect of Phenyl ring should hypothetically have destabilizing effect on **TS-3a-r** and stabilizing effect on **TS-3b-r**. Whereas increasing -M effect should stabilize **TS-3a-r** and destabilize **TS-3b-r**. A proof of concept is shown here where +M effect of phenyl ring is increased by introducing NMe₂ and -M effect is increased by introducing CN group. Predicted barriers are consistent with the hypothesis.

Table 7. Cartesian coordinates (xyz format) and energies of all the structures involved in each reaction mechanism studied calculated at the UB3LYP-d3/def2-svp/CPCM(THF) level of theory.

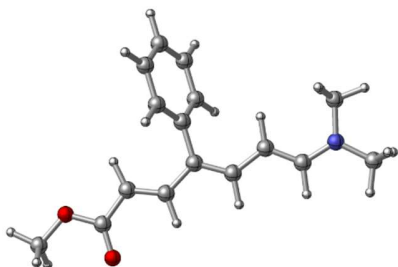
3a

E(scf) = -825.763525522 a.u.

$\nu_{\min} = 28.2 \text{ cm}^{-1}$

C	-0.152966	2.218025	0.394035	C	-4.641762	0.636588	-0.624015
C	-1.490052	2.570486	0.384228	O	-4.267301	-0.487377	-0.917740
C	-2.456947	1.591783	-0.039532	O	-5.947263	1.000132	-0.694817
H	0.080337	1.199584	0.057535	C	2.242256	2.516746	0.757333
H	-2.059395	0.604221	-0.303555	H	2.401160	1.495797	0.393730
C	-3.805383	1.745323	-0.165897	H	0.768336	4.023288	1.166674
H	-4.306323	2.687206	0.062688	C	-6.860571	-0.002968	-1.132403
C	0.955235	3.010912	0.805123	H	-6.609026	-0.354195	-2.145835

H	-6.850837	-0.871536	-0.454762	C	-1.940947	3.934210	0.795148
H	-7.854899	0.461429	-1.132355	C	-2.796052	4.109873	1.898887
N	3.368452	3.165006	1.114677	C	-1.523225	5.076809	0.088606
C	3.303884	4.527297	1.616489	C	-3.216047	5.385647	2.286404
H	2.829114	5.197374	0.879800	H	-3.130997	3.233037	2.458437
H	2.720122	4.581688	2.552127	C	-1.940907	6.354151	0.474970
H	4.318512	4.893450	1.816619	H	-0.864054	4.956593	-0.774746
C	4.669740	2.519381	1.062739	C	-2.789558	6.513378	1.575825
H	5.365404	3.087957	0.422529	H	-3.877534	5.499955	3.149330
H	5.115420	2.442831	2.069793	H	-1.605407	7.228425	-0.089322
H	4.570038	1.506288	0.651074	H	-3.117985	7.511144	1.878120



Zero-point correction=	0.316565 (Hartree/Particle)
Thermal correction to Energy=	0.336293
Thermal correction to Enthalpy=	0.337238
Thermal correction to Gibbs Free Energy=	0.265520
Sum of electronic and zero-point Energies=	-825.446961
Sum of electronic and thermal Energies=	-825.427232
Sum of electronic and thermal Enthalpies=	-825.426288
Sum of electronic and thermal Free Energies=	-825.498005

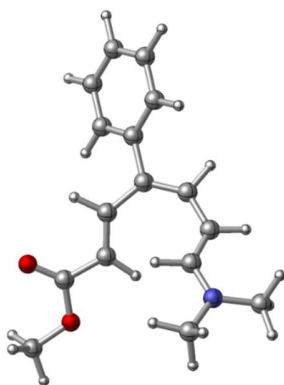
3a-aii

E(scf) = -825.746690573 a.u.

$\nu_{\min} = 11.5 \text{ cm}^{-1}$

C	-0.173573	4.200421	0.503584	C	0.960023	3.439053	0.940974
C	-1.548347	4.024016	0.564765	C	-2.813644	0.412288	1.076044
C	-2.264934	2.794627	0.877222	O	-3.953522	0.530887	1.490965
H	0.127159	5.143281	0.031168	O	-2.250826	-0.798045	0.844285
H	-3.308775	2.928601	1.185443	C	0.961033	2.449742	1.900833
C	-1.877206	1.497853	0.764405	H	0.019630	2.166545	2.375464
H	-0.883914	1.204256	0.423492	H	1.918814	3.768163	0.533200

C	-3.068940	-1.937302	1.105146	H	0.853973	0.678827	3.707754
H	-3.377242	-1.968869	2.162146	C	-2.413120	5.190694	0.219312
H	-3.976324	-1.923716	0.480901	C	-3.627484	5.018645	-0.480920
H	-2.459957	-2.817670	0.864295	C	-2.052775	6.508280	0.576788
N	2.033346	1.778318	2.362742	C	-4.435294	6.108633	-0.814622
C	3.361990	2.048774	1.840049	H	-3.933338	4.017017	-0.792912
H	4.086510	1.373317	2.311507	C	-2.854988	7.599974	0.235489
H	3.395820	1.892797	0.748518	H	-1.141429	6.676070	1.155664
H	3.667092	3.089601	2.045807	C	-4.053002	7.407574	-0.461570
C	1.906809	0.780720	3.413352	H	-5.365731	5.941857	-1.364187
H	2.267529	-0.202571	3.066718	H	-2.549405	8.607259	0.531549
H	2.493034	1.067348	4.303361	H	-4.684612	8.260496	-0.722559



Zero-point correction=	0.316582 (Hartree/Particle)
Thermal correction to Energy=	0.336314
Thermal correction to Enthalpy=	0.337258
Thermal correction to Gibbs Free Energy=	0.265004
Sum of electronic and zero-point Energies=	-825.430108
Sum of electronic and thermal Energies=	-825.410377
Sum of electronic and thermal Enthalpies=	-825.409433
Sum of electronic and thermal Free Energies=	-825.481687

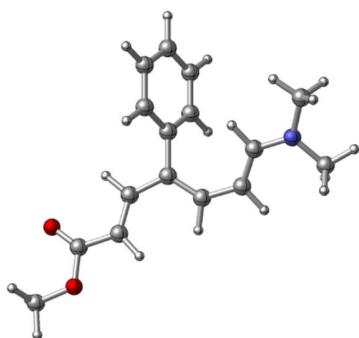
3a-int

E(scf) = -825.751749528 a.u.

$\nu_{\min} = 22.2 \text{ cm}^{-1}$

C	-0.208691	1.951213	0.683882	C	-1.502571	2.411250	0.518978
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C	-2.546271	1.551966	-0.002603	C	3.362785	3.671937	2.473028
H	-0.016470	0.953852	0.272126	H	4.105260	4.330641	2.940791
H	-3.484816	2.055159	-0.263723	H	3.484029	2.655750	2.888749
C	-2.535066	0.204599	-0.205788	H	3.568786	3.625159	1.391108
H	-1.684423	-0.426992	0.058137	C	1.886624	5.259527	3.696638
C	0.944934	2.534220	1.299456	H	2.194610	4.925232	4.703081
C	-3.697786	-0.469914	-0.784409	H	2.509019	6.125733	3.417486
O	-4.746369	0.049152	-1.130241	H	0.839132	5.585657	3.743963
O	-3.484899	-1.805308	-0.897897	C	-1.911580	3.814914	0.832223
C	0.949300	3.626556	2.144711	C	-2.926104	4.081778	1.768172
H	0.003430	4.102011	2.409300	C	-1.311877	4.904581	0.170989
H	1.887189	2.013876	1.113684	C	-3.316738	5.396049	2.051416
C	-4.553828	-2.571624	-1.447952	H	-3.406265	3.247667	2.286893
H	-5.463642	-2.481913	-0.833368	C	-1.698748	6.215852	0.451948
H	-4.794726	-2.239440	-2.470331	H	-0.525730	4.711135	-0.563037
H	-4.212232	-3.614398	-1.463017	C	-2.701365	6.467943	1.398207
N	2.028263	4.190658	2.720639	H	-4.103691	5.581294	2.787386



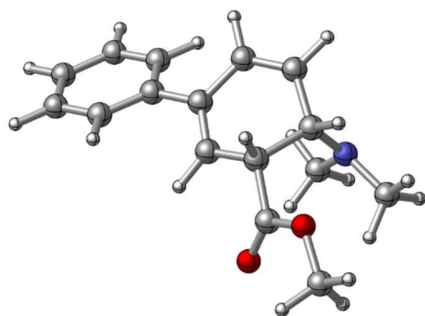
Zero-point correction=	0.316368 (Hartree/Particle)
Thermal correction to Energy=	0.336168
Thermal correction to Enthalpy=	0.337112
Thermal correction to Gibbs Free Energy=	0.265146
Sum of electronic and zero-point Energies=	-825.435382
Sum of electronic and thermal Energies=	-825.415582
Sum of electronic and thermal Enthalpies=	-825.414638
Sum of electronic and thermal Free Energies=	-825.486603

3a-p1

E(scf) = -825.757528762 a.u.

$\nu_{\min} = 40.6 \text{ cm}^{-1}$

C	-1.393976	4.525141	0.936676	C	-4.407689	4.215568	2.619988
C	-1.135614	3.383502	1.834733	H	-4.368591	3.223687	3.119013
C	-1.956124	2.308280	1.760330	H	-3.440195	4.711323	2.780212
H	-1.875856	1.477710	2.464381	H	-5.183500	4.815580	3.123267
C	-3.002673	2.224344	0.690579	C	-6.059206	3.668059	0.933114
H	-2.500846	1.932722	-0.252712	H	-6.293247	2.671945	1.365487
C	-2.540430	4.642472	0.239966	H	-6.784429	4.380431	1.361849
C	-4.046104	1.160177	0.956417	H	-6.236728	3.614509	-0.151073
O	-4.233764	0.596435	2.011343	H	-0.638006	5.312421	0.872592
O	-4.771776	0.917132	-0.146590	C	-0.036344	3.471254	2.829688
C	-3.652305	3.617290	0.339384	C	0.686906	2.325449	3.218169
H	-4.102810	3.494877	-0.655778	C	0.306160	4.701825	3.425110
H	-2.744894	5.535085	-0.357438	C	1.701867	2.404159	4.174072
C	-5.835105	-0.033260	-0.023577	H	0.462370	1.365402	2.747836
H	-5.448508	-1.010570	0.301420	C	1.322665	4.781300	4.381219
H	-6.581077	0.313213	0.708212	H	-0.243564	5.606335	3.154530
H	-6.290318	-0.114029	-1.017716	C	2.025290	3.633075	4.761184
N	-4.706660	4.123644	1.202855	H	2.251740	1.501835	4.454331



Zero-point correction= 0.319044 (Hartree/Particle)
 Thermal correction to Energy= 0.336971
 Thermal correction to Enthalpy= 0.337915
 Thermal correction to Gibbs Free Energy= 0.272811
 Sum of electronic and zero-point Energies= -825.438484
 Sum of electronic and thermal Energies= -825.420558
 Sum of electronic and thermal Enthalpies= -825.419614
 Sum of electronic and thermal Free Energies= -825.484718

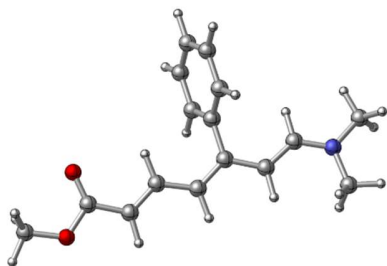
3b

E(scf) = -825.761853779 a.u.

$\nu_{\min} = 24.1 \text{ cm}^{-1}$

C	0.190017	2.624312	-0.750587	C	-1.179429	2.482494	-0.881058
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C	-2.041593	1.823772	0.046585	H	1.755939	5.302180	-3.786216
H	-1.593803	1.372441	0.938195	H	3.312359	4.890994	-4.561406
C	-3.394212	1.698709	-0.081977	C	4.472162	4.440949	-2.372995
H	-3.931797	2.119976	-0.935339	H	5.130767	3.991926	-3.135549
C	0.962979	3.252476	-1.788425	H	4.633445	5.533495	-2.381674
C	-4.181011	0.992023	0.927062	H	4.770622	4.056411	-1.388606
O	-3.755298	0.461102	1.940405	H	-1.645467	2.892543	-1.784683
O	-5.500972	0.984057	0.611554	C	0.888398	2.127049	0.475976
C	2.307231	3.534850	-1.688491	C	0.649722	2.719329	1.727984
H	2.836852	3.280652	-0.766646	C	1.798170	1.057486	0.398299
H	0.417654	3.537808	-2.691213	C	1.301425	2.253101	2.873915
C	-6.366137	0.320607	1.529821	H	-0.053281	3.552747	1.798071
H	-6.095651	-0.742351	1.633228	C	2.445164	0.586907	1.544413
H	-6.318715	0.786084	2.527242	H	1.991235	0.589722	-0.570155
H	-7.380678	0.411451	1.121367	C	2.199737	1.184473	2.785897
N	3.080614	4.111830	-2.632763	H	1.105351	2.726647	3.839326
C	2.515817	4.509932	-3.909989	H	3.142423	-0.251415	1.467825
H	2.035313	3.653281	-4.412041	H	2.706963	0.817791	3.681898



Zero-point correction=	0.316297 (Hartree/Particle)
Thermal correction to Energy=	0.336109
Thermal correction to Enthalpy=	0.337054
Thermal correction to Gibbs Free Energy=	0.265006
Sum of electronic and zero-point Energies=	-825.445557
Sum of electronic and thermal Energies=	-825.425744
Sum of electronic and thermal Enthalpies=	-825.424800
Sum of electronic and thermal Free Energies=	-825.496847

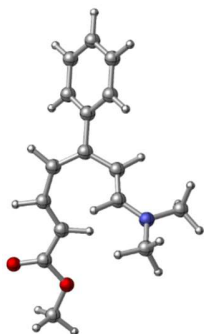
3b-aii

E(scf) = -825.749051404 a.u.

$\nu_{\min} = 29.7 \text{ cm}^{-1}$

C	-0.893350	4.880610	1.559728	C	-0.244305	3.654799	1.535693
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C	-0.629296	2.347506	2.006757	H	-5.075655	6.382819	1.668084
H	0.132145	1.578129	1.826626	H	-6.243244	5.229887	2.378995
C	-1.706302	1.895917	2.712260	C	-5.514035	3.473435	0.694347
H	-2.556848	2.522218	2.977363	H	-6.281530	3.047412	1.360437
C	-2.311965	5.096148	1.750487	H	-6.027272	4.038181	-0.105027
C	-1.752211	0.508277	3.177325	H	-4.958230	2.646786	0.231867
O	-0.928430	-0.365670	2.963310	H	0.784000	3.680957	1.163819
O	-2.872969	0.275753	3.907142	C	-0.070455	6.109585	1.352357
C	-3.268205	4.231033	1.278961	C	1.240074	6.211014	1.862884
H	-2.945473	3.360653	0.701230	C	-0.590659	7.212497	0.644634
H	-2.615765	6.045877	2.196277	C	2.004057	7.362816	1.662208
C	-3.032815	-1.045928	4.417037	H	1.652859	5.385111	2.446306
H	-3.079180	-1.783383	3.599925	C	0.173879	8.363482	0.440195
H	-2.196795	-1.319161	5.080323	H	-1.600139	7.153424	0.231756
H	-3.975031	-1.049592	4.979646	C	1.475428	8.444002	0.947842
N	-4.603918	4.322722	1.445746	H	3.014434	7.420798	2.075367
C	-5.176520	5.420930	2.203688	H	-0.247266	9.200632	-0.122682
H	-4.673472	5.518198	3.178842	H	2.072691	9.346039	0.792131



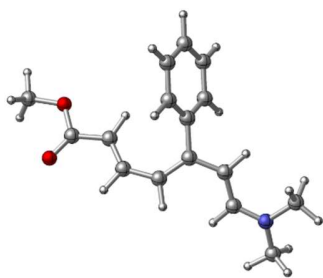
Zero-point correction= 0.316777 (Hartree/Particle)
 Thermal correction to Energy= 0.336358
 Thermal correction to Enthalpy= 0.337302
 Thermal correction to Gibbs Free Energy= 0.266572
 Sum of electronic and zero-point Energies= -825.432274
 Sum of electronic and thermal Energies= -825.412693
 Sum of electronic and thermal Enthalpies= -825.411749
 Sum of electronic and thermal Free Energies= -825.482479

3b-int

E(scf) = -825.750949451 a.u.

 $\nu_{\min} = 22.7 \text{ cm}^{-1}$

C	-2.274478	4.252784	1.252468	H	-5.138204	7.389518	-0.079179
C	-2.303673	2.869232	1.261230	H	-4.243597	6.683457	-1.454852
C	-1.542640	1.934934	2.048135	H	-5.999755	6.973647	-1.589657
H	-1.671765	0.885403	1.755750	C	-6.849552	4.855055	-0.473211
C	-0.725874	2.123651	3.124142	H	-7.501797	5.451686	0.190439
H	-0.525858	3.104964	3.552306	H	-7.243931	4.930788	-1.499324
C	-3.272043	5.068091	0.597612	H	-6.904144	3.804882	-0.155872
C	-0.080697	0.980908	3.772509	H	-3.030453	2.394134	0.595686
O	-0.165626	-0.191952	3.446631	C	-1.165246	5.018815	1.897900
O	0.663666	1.378639	4.835589	C	0.168394	4.817812	1.499763
C	-4.532476	4.629417	0.260066	C	-1.437272	5.981413	2.884716
H	-4.847895	3.627570	0.568140	C	1.204148	5.547764	2.085217
H	-3.000248	6.108761	0.410250	H	0.385655	4.073902	0.729887
C	1.341704	0.350719	5.553362	C	-0.398896	6.703924	3.481881
H	0.629281	-0.380298	5.967795	H	-2.471711	6.152162	3.193227
H	2.048112	-0.188310	4.902136	C	0.924675	6.488867	3.084281
H	1.885580	0.847292	6.366977	H	2.235228	5.381896	1.762350
N	-5.472276	5.318232	-0.422924	H	-0.625533	7.438767	4.258767
C	-5.198979	6.659426	-0.907358	H	1.736402	7.055961	3.547048



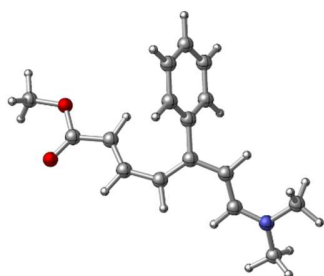
Zero-point correction=	0.316329 (Hartree/Particle)
Thermal correction to Energy=	0.336064
Thermal correction to Enthalpy=	0.337008
Thermal correction to Gibbs Free Energy=	0.265442
Sum of electronic and zero-point Energies=	-825.434621
Sum of electronic and thermal Energies=	-825.414885
Sum of electronic and thermal Enthalpies=	-825.413941
Sum of electronic and thermal Free Energies=	-825.485507

3b-p1

E(scf) = -825.756268226 a.u.

 $\nu_{\min} = 38.5 \text{ cm}^{-1}$

C	-1.523942	4.619074	1.229361	H	-4.774392	3.400492	3.086952
C	-1.404978	3.505725	2.188748	H	-3.813136	4.872823	2.773163
C	-2.181687	2.412497	2.091594	H	-5.587091	4.979609	2.874491
H	-2.126205	1.604340	2.824277	C	-6.160297	3.686182	0.666010
C	-3.104150	2.253044	0.919154	H	-6.457654	2.722792	1.132140
H	-2.497492	1.892149	0.066396	H	-6.934460	4.423946	0.937976
C	-2.589203	4.658372	0.390439	H	-6.186597	3.553957	-0.425676
C	-4.183112	1.213954	1.135595	H	-0.670606	3.583683	2.993291
O	-4.515027	0.746942	2.202141	C	-0.508539	5.707188	1.242294
O	-4.757420	0.871329	-0.028550	C	0.046313	6.174716	2.449737
C	-3.691750	3.620603	0.404546	C	-0.084402	6.309952	0.041632
H	-4.006656	3.439313	-0.633407	C	0.977320	7.217193	2.457043
H	-2.763250	5.529932	-0.245691	H	-0.269728	5.737359	3.399444
C	-5.835894	-0.067828	0.034893	C	0.847490	7.350524	0.048197
H	-5.505447	-1.009883	0.497014	H	-0.478267	5.942716	-0.908895
H	-6.671261	0.341154	0.623901	C	1.382707	7.810277	1.256750
H	-6.152824	-0.240779	-1.000346	H	1.385546	7.569963	3.407766
N	-4.856020	4.166746	1.086130	H	1.165155	7.798037	-0.897244
C	-4.749614	4.356004	2.520845	H	2.114649	8.621879	1.262465



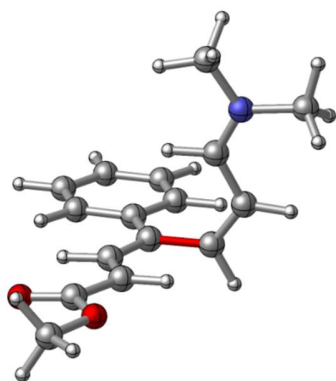
Zero-point correction=	0.319005 (Hartree/Particle)
Thermal correction to Energy=	0.336951
Thermal correction to Enthalpy=	0.337895
Thermal correction to Gibbs Free Energy=	0.272782
Sum of electronic and zero-point Energies=	-825.437264
Sum of electronic and thermal Energies=	-825.419317
Sum of electronic and thermal Enthalpies=	-825.418373
Sum of electronic and thermal Free Energies=	-825.483487

TS-3a-r

E(scf) = -825.709631147 a.u.

 $\nu_{\min} = -511.0 \text{ cm}^{-1}$

C	-0.287755	3.316329	-0.435546	C	2.970572	2.677126	2.277928
C	-1.682626	3.437751	0.053349	H	3.571048	2.645601	3.193524
C	-2.398208	2.251729	0.208041	H	3.190725	1.785728	1.672448
H	-0.099146	3.379086	-1.519121	H	3.231575	3.579620	1.709489
H	-3.451115	2.332174	0.499715	C	1.223219	2.448001	4.047623
C	-1.941654	0.937062	0.058786	H	1.620718	1.464782	4.340663
H	-0.909018	0.712049	-0.214272	H	1.688989	3.222578	4.674698
C	0.800413	3.094336	0.353161	H	0.136627	2.461453	4.191336
C	-2.823761	-0.171263	0.274827	C	-2.214084	4.776571	0.288969
O	-4.012428	-0.141433	0.596283	C	-3.537507	5.011326	0.755364
O	-2.186576	-1.380036	0.086764	C	-1.418607	5.932678	0.059454
C	0.607738	2.901765	1.756962	C	-4.019213	6.299926	0.972494
H	-0.425546	2.910500	2.118745	H	-4.198869	4.166364	0.956390
H	1.796190	3.012669	-0.085989	C	-1.907212	7.221672	0.280707
C	-2.980370	-2.539022	0.280120	H	-0.392109	5.816882	-0.298599
H	-3.376056	-2.596416	1.308330	C	-3.213344	7.425019	0.739744
H	-3.840138	-2.564826	-0.410497	H	-5.044060	6.429951	1.333354
H	-2.328309	-3.402599	0.088229	H	-1.255258	8.079347	0.088863
N	1.546115	2.699784	2.640754	H	-3.596579	8.433498	0.913079



Zero-point correction= 0.314604 (Hartree/Particle)
Thermal correction to Energy= 0.333973
Thermal correction to Enthalpy= 0.334917
Thermal correction to Gibbs Free Energy= 0.263999
Sum of electronic and zero-point Energies= -825.395027

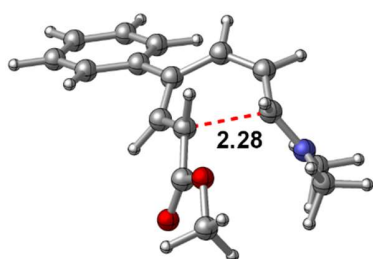
Sum of electronic and thermal Energies= -825.375658
 Sum of electronic and thermal Enthalpies= -825.374714
 Sum of electronic and thermal Free Energies= -825.445632

TS-3a-uu

E(scf) = -825.722678629 a.u.

$\nu_{\min} = -268.29 \text{ cm}^{-1}$

C	-1.495684	4.504547	1.301991	H	-5.808306	4.237914	3.086542
C	-1.038586	3.316276	1.974658	H	-4.243093	5.064986	2.813453
C	-1.834935	2.176127	1.964462	H	-5.764527	5.811701	2.242369
H	-1.787844	1.474242	2.805855	C	-6.293145	3.561027	0.576351
C	-2.781768	1.943295	0.946054	H	-6.718103	2.833805	1.290341
H	-2.471224	2.141071	-0.078954	H	-7.052515	4.338402	0.388437
C	-2.751051	4.792529	0.815485	H	-6.073633	3.039463	-0.363287
C	-3.840507	0.955502	1.121064	H	-0.824250	5.366975	1.357438
O	-4.151745	0.402581	2.162566	C	0.153994	3.384376	2.855392
O	-4.522771	0.745285	-0.038814	C	0.918313	2.222200	3.100279
C	-3.876259	3.905138	0.563797	C	0.562704	4.575613	3.494737
H	-3.943018	3.381362	-0.386366	C	2.027199	2.245119	3.949708
H	-3.004777	5.858451	0.744064	H	0.647200	1.291792	2.595630
C	-5.635566	-0.142548	0.033334	C	1.679004	4.602197	4.333831
H	-5.326772	-1.139679	0.383378	H	-0.016102	5.491611	3.357828
H	-6.404394	0.243234	0.722390	C	2.417921	3.436926	4.569684
H	-6.045012	-0.209981	-0.982516	H	2.598696	1.327924	4.116343
N	-5.079640	4.154375	1.115348	H	1.966274	5.539379	4.818422
C	-5.229293	4.856743	2.379736	H	3.289991	3.458680	5.228135



Zero-point correction= 0.315729 (Hartree/Particle)
 Thermal correction to Energy= 0.334345
 Thermal correction to Enthalpy= 0.335289
 Thermal correction to Gibbs Free Energy= 0.267895
 Sum of electronic and zero-point Energies= -825.406950

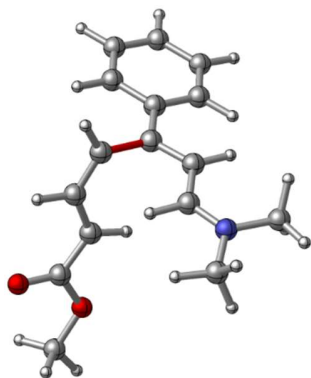
Sum of electronic and thermal Energies= -825.388333
 Sum of electronic and thermal Enthalpies= -825.387389
 Sum of electronic and thermal Free Energies= -825.454784

TS-3b-r

E(scf) = -825.708129187 a.u.

$\nu_{\min} = -616.9 \text{ cm}^{-1}$

C	-1.535890	4.847069	0.936048	H	-5.225962	6.626015	0.332797
C	-1.126704	3.523600	0.402169	H	-6.795428	5.822143	0.610691
C	-1.148623	2.380361	1.164573	H	-5.631284	5.985947	1.957883
H	-0.809618	1.455633	0.680123	C	-6.094965	3.454261	0.158518
C	-1.587200	2.227105	2.499703	H	-6.777039	3.272597	1.003378
H	-1.953104	3.082146	3.073254	H	-6.689029	3.755518	-0.717544
C	-2.866816	5.223912	0.942148	H	-5.548196	2.531588	-0.069332
C	-1.571211	0.955959	3.135626	H	-0.804497	3.498913	-0.643250
O	-1.207496	-0.131315	2.673297	C	-0.502374	5.751852	1.484249
O	-2.043321	1.019419	4.441174	C	0.748398	5.221167	1.869589
C	-3.859818	4.298685	0.536290	C	-0.710378	7.142552	1.632738
H	-3.517871	3.303837	0.235835	C	1.737774	6.040296	2.411953
H	-3.173225	6.190755	1.341508	H	0.918737	4.150649	1.747472
C	-2.061311	-0.203626	5.151874	C	0.289190	7.963782	2.152097
H	-2.706637	-0.955342	4.664866	H	-1.649768	7.596397	1.312468
H	-1.053097	-0.644020	5.241884	C	1.514653	7.415442	2.551349
H	-2.453214	0.018729	6.155061	H	2.691659	5.606156	2.721174
N	-5.154270	4.518749	0.508082	H	0.114504	9.038624	2.242670
C	-5.731927	5.815455	0.875055	H	2.295595	8.060233	2.962186



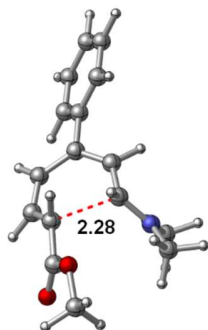
Zero-point correction= 0.314159 (Hartree/Particle)
 Thermal correction to Energy= 0.333604
 Thermal correction to Enthalpy= 0.334548
 Thermal correction to Gibbs Free Energy= 0.263025
 Sum of electronic and zero-point Energies= -825.393970
 Sum of electronic and thermal Energies= -825.374525
 Sum of electronic and thermal Enthalpies= -825.373581
 Sum of electronic and thermal Free Energies= -825.445104

TS-3b-uu

E(scf) = -825.719525678 a.u.

$\nu_{\min} = -292.22 \text{ cm}^{-1}$

C	-1.422207	4.469523	1.262841	H	-5.858497	4.350218	2.953609
C	-1.050753	3.254791	1.934769	H	-4.237883	5.082347	2.744770
C	-1.856240	2.138812	1.988745	H	-5.684457	5.904458	2.090813
H	-1.771928	1.447589	2.836894	C	-6.254479	3.631609	0.447019
C	-2.838093	1.891962	1.000525	H	-6.743678	2.944641	1.160183
H	-2.533585	2.014737	-0.037058	H	-6.971824	4.432910	0.200716
C	-2.694107	4.757677	0.778512	H	-6.016730	3.071576	-0.465742
C	-3.927736	0.954629	1.242733	H	-0.162511	3.296482	2.569903
O	-4.238969	0.465902	2.316173	C	-0.456403	5.612467	1.302562
O	-4.641882	0.715042	0.107875	C	0.325462	5.896350	2.439683
C	-3.824932	3.889596	0.518610	C	-0.319333	6.453417	0.180951
H	-3.879914	3.343473	-0.419172	C	1.207850	6.979433	2.453586
H	-2.952787	5.823688	0.751424	H	0.225524	5.279466	3.335231
C	-5.791171	-0.115824	0.247735	C	0.565620	7.535508	0.192317
H	-5.519698	-1.108513	0.639110	H	-0.904805	6.240031	-0.716466
H	-6.524687	0.337449	0.934333	C	1.334122	7.803656	1.329472
H	-6.228258	-0.212651	-0.754161	H	1.795374	7.185346	3.352183
N	-5.042100	4.189452	1.022262	H	0.658853	8.167788	-0.694602
C	-5.212285	4.922239	2.265601	H	2.027205	8.648700	1.340639



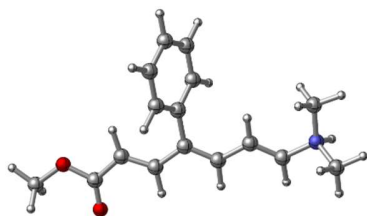
Zero-point correction= 0.315467 (Hartree/Particle)
 Thermal correction to Energy= 0.334150
 Thermal correction to Enthalpy= 0.335094
 Thermal correction to Gibbs Free Energy= 0.267470
 Sum of electronic and zero-point Energies= -825.404059
 Sum of electronic and thermal Energies= -825.385376
 Sum of electronic and thermal Enthalpies= -825.384431
 Sum of electronic and thermal Free Energies= -825.452055

3a-H

E(scf) = -826.181186664 a.u.

$\nu_{\min} = 28.74 \text{ cm}^{-1}$

C	-0.100630	2.121677	0.156164	C	3.186094	4.749639	1.227306
C	-1.414551	2.480055	0.270974	H	2.600026	5.291182	0.476625
C	-2.430593	1.511614	-0.126944	H	2.633451	4.675952	2.170438
H	0.131264	1.132252	-0.250337	H	4.143917	5.254345	1.395240
H	-2.073149	0.522098	-0.431991	C	4.334006	2.596645	1.692239
C	-3.762562	1.726257	-0.172166	H	5.252871	3.166998	1.875443
H	-4.211911	2.682400	0.100990	H	3.765201	2.465830	2.620092
C	1.021744	2.948595	0.545371	H	4.575716	1.621853	1.252566
C	-4.679299	0.649587	-0.612296	C	-1.832527	3.824730	0.764388
O	-4.347135	-0.470899	-0.943401	C	-2.597964	3.950874	1.937778
O	-5.954827	1.070811	-0.602892	C	-1.468357	4.987801	0.062812
C	2.292326	2.573980	0.328944	C	-2.977676	5.211914	2.403817
H	2.569680	1.635441	-0.154477	H	-2.888780	3.054312	2.490004
H	0.792890	3.899527	1.029379	C	-1.854033	6.248721	0.527589
C	-6.944789	0.121905	-1.012593	H	-0.887706	4.898542	-0.858593
H	-6.761951	-0.209383	-2.046272	C	-2.607596	6.363818	1.700023
H	-6.934520	-0.760015	-0.354012	H	-3.565275	5.295470	3.321328
H	-7.910491	0.636512	-0.943665	H	-1.567707	7.143081	-0.031248
N	3.472675	3.367606	0.722312	H	-2.909134	7.349071	2.063941



Zero-point correction= 0.332185 (Hartree/Particle)
 Thermal correction to Energy= 0.351576
 Thermal correction to Enthalpy= 0.352520

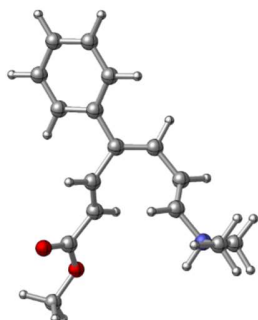
Thermal correction to Gibbs Free Energy=	0.282131
Sum of electronic and zero-point Energies=	-825.849002
Sum of electronic and thermal Energies=	-825.829611
Sum of electronic and thermal Enthalpies=	-825.828667
Sum of electronic and thermal Free Energies=	-825.899056

3a-H-aii

E(scf) = -826.167461541 a.u.

$\nu_{\min} = 27.35 \text{ cm}^{-1}$

C	-0.169656	3.157630	0.683134	C	2.591542	-0.208678	0.981846
C	-1.530105	3.184716	0.707329	H	3.137063	-1.134706	1.195941
C	-2.376305	1.974035	0.790506	H	2.183226	-0.237112	-0.034334
H	0.348627	4.100267	0.482271	H	3.256852	0.652395	1.109304
H	-3.178044	1.978814	1.538900	C	1.966547	-0.128698	3.382416
C	-2.296536	0.913914	-0.029881	H	2.553914	-1.042914	3.529268
H	-1.555628	0.856258	-0.830461	H	2.586594	0.761492	3.539010
C	0.733851	2.022620	0.880179	H	1.107138	-0.117384	4.062852
C	-3.222270	-0.234198	0.126597	C	-2.268404	4.473869	0.624005
O	-4.092128	-0.329264	0.967654	C	-3.532964	4.526097	0.003983
O	-2.974592	-1.179862	-0.794216	C	-1.737321	5.664124	1.161635
C	0.540043	1.033728	1.759272	C	-4.232091	5.731222	-0.095828
H	-0.329198	0.970603	2.414444	H	-3.965339	3.617801	-0.421876
H	1.652286	2.057728	0.287697	C	-2.437914	6.866980	1.062885
C	-3.808223	-2.343447	-0.755950	H	-0.779020	5.643170	1.685116
H	-3.711068	-2.859952	0.211230	C	-3.686809	6.906356	0.431330
H	-4.863996	-2.069890	-0.903705	H	-5.206871	5.751914	-0.589191
H	-3.466317	-2.993015	-1.570342	H	-2.012076	7.777330	1.491969
N	1.462656	-0.101344	1.961091	H	-4.235682	7.848373	0.357971



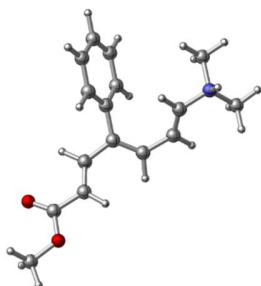
Zero-point correction= 0.331809 (Hartree/Particle)
 Thermal correction to Energy= 0.351290
 Thermal correction to Enthalpy= 0.352234
 Thermal correction to Gibbs Free Energy= 0.281721
 Sum of electronic and zero-point Energies= -825.835652
 Sum of electronic and thermal Energies= -825.816172
 Sum of electronic and thermal Enthalpies= -825.815228
 Sum of electronic and thermal Free Energies= -825.885740

3a-H-int

E(scf) = -826.170479003 a.u.

$\nu_{\min} = 30.83 \text{ cm}^{-1}$

C	-0.534773	0.856537	0.206425	C	3.092720	1.362459	2.599365
C	-1.654864	1.626429	0.115023	H	3.862818	1.590510	3.345139
C	-2.811524	1.189627	-0.680483	H	2.978108	0.277768	2.495821
H	-0.476105	-0.035915	-0.423725	H	3.357391	1.818292	1.638765
H	-3.446712	1.979792	-1.095557	C	1.908521	3.438546	3.283248
C	-3.185731	-0.085242	-0.905978	H	2.723267	3.634892	3.990500
H	-2.652502	-0.938037	-0.479702	H	2.113568	3.901102	2.310849
C	0.646855	1.089526	1.037210	H	0.957952	3.811128	3.682609
C	-4.377687	-0.384796	-1.735342	C	-1.786067	2.967560	0.759943
O	-5.095241	0.438960	-2.264671	C	-2.864848	3.237055	1.618798
O	-4.575823	-1.709944	-1.828823	C	-0.846284	3.983763	0.509324
C	0.610801	1.642941	2.255234	C	-2.982174	4.484075	2.241925
H	-0.308854	1.972566	2.738890	H	-3.608165	2.459206	1.811592
H	1.592796	0.735721	0.618358	C	-0.968111	5.230319	1.125410
C	-5.701852	-2.135054	-2.603771	H	-0.014696	3.787453	-0.171293
H	-6.637151	-1.738272	-2.180284	C	-2.032566	5.481806	2.000527
H	-5.611679	-1.787197	-3.644157	H	-3.820123	4.675961	2.916529
H	-5.703078	-3.230877	-2.567999	H	-0.232204	6.011500	0.918925
N	1.798231	1.946723	3.076098	H	-2.126107	6.457126	2.484328



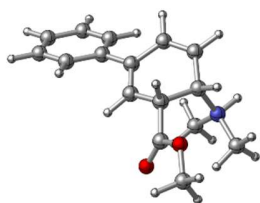
Zero-point correction=	0.331925 (Hartree/Particle)
Thermal correction to Energy=	0.351354
Thermal correction to Enthalpy=	0.352298
Thermal correction to Gibbs Free Energy=	0.282042
Sum of electronic and zero-point Energies=	-825.838554
Sum of electronic and thermal Energies=	-825.819125
Sum of electronic and thermal Enthalpies=	-825.818181
Sum of electronic and thermal Free Energies=	-825.888437

3a-H-p1

E(scf) = -826.202040660 a.u.

$\nu_{\min} = 40.68 \text{ cm}^{-1}$

C	-1.379254	4.532644	0.920408	H	-4.357931	3.172361	3.009820
C	-1.158093	3.400937	1.839799	H	-3.430730	4.703947	2.818643
C	-1.998861	2.344747	1.756659	H	-5.184249	4.757602	3.202198
H	-1.923383	1.494842	2.436279	C	-6.092193	3.643709	0.959184
C	-3.048624	2.280473	0.680948	H	-6.151146	2.652108	1.417586
H	-2.545163	1.954861	-0.250211	H	-6.832499	4.300629	1.430943
C	-2.502768	4.669919	0.190984	H	-6.275134	3.583522	-0.119292
C	-4.124483	1.236054	0.948204	H	-0.597241	5.291000	0.837825
O	-4.392712	0.784603	2.038035	C	-0.055618	3.472097	2.831509
O	-4.758497	0.911089	-0.178075	C	0.640486	2.313107	3.226838
C	-3.615018	3.656961	0.276868	C	0.308237	4.701741	3.413949
H	-4.119088	3.557582	-0.692086	C	1.656887	2.380256	4.181535
H	-2.650939	5.532101	-0.464124	H	0.398057	1.353585	2.764631
C	-5.821918	-0.052654	-0.078827	C	1.324788	4.767877	4.370584
H	-5.445491	-0.993210	0.347374	H	-0.220972	5.616288	3.135456
H	-6.631448	0.332101	0.559276	C	2.002792	3.607809	4.758404
H	-6.183743	-0.208716	-1.100927	H	2.189489	1.470358	4.469137
N	-4.729268	4.223204	1.204469	H	1.585693	5.730796	4.816598
C	-4.396669	4.212375	2.668023	H	2.801187	3.660131	5.502620



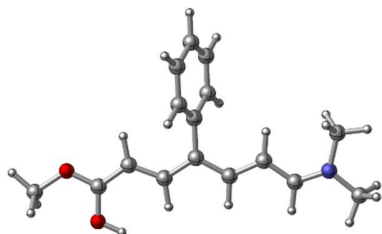
Zero-point correction= 0.335181 (Hartree/Particle)
 Thermal correction to Energy= 0.353021
 Thermal correction to Enthalpy= 0.353965
 Thermal correction to Gibbs Free Energy= 0.289026
 Sum of electronic and zero-point Energies= -825.866860
 Sum of electronic and thermal Energies= -825.849020
 Sum of electronic and thermal Enthalpies= -825.848076
 Sum of electronic and thermal Free Energies= -825.913015

3a-OH'

E(scf) = -826.190534011 a.u.

$\nu_{\min} = 28.85 \text{ cm}^{-1}$

C	-0.116021	2.185927	0.381171	C	3.253286	4.535185	1.659827
C	-1.482376	2.537235	0.356773	H	2.805412	5.201375	0.906399
C	-2.407354	1.574156	-0.067462	H	2.638736	4.568517	2.572915
H	0.131063	1.173181	0.039960	H	4.260009	4.896836	1.897619
H	-1.975334	0.601252	-0.334595	C	4.667124	2.562146	1.078972
C	-3.790810	1.743338	-0.187946	H	5.320680	3.158901	0.423369
H	-4.257010	2.698500	0.053099	H	5.118380	2.523875	2.082961
C	0.941585	2.990215	0.802755	H	4.595515	1.542659	0.680179
C	-4.666864	0.746410	-0.615679	C	-1.928897	3.901350	0.773813
O	-4.353689	-0.491954	-0.951866	C	-2.709815	4.078292	1.929242
O	-5.942651	1.031575	-0.703604	C	-1.572692	5.032775	0.018924
C	2.255390	2.507069	0.771388	C	-3.124635	5.354912	2.320214
H	2.431810	1.490804	0.404460	H	-2.990263	3.206374	2.525469
H	0.734524	3.999718	1.159633	C	-1.986555	6.309486	0.410110
C	-6.882979	0.031132	-1.139476	H	-0.968524	4.907123	-0.883096
H	-6.641297	-0.303569	-2.158223	C	-2.763723	6.473915	1.561927
H	-6.873119	-0.828426	-0.454475	H	-3.729685	5.475937	3.222298
H	-7.860862	0.523889	-1.120826	H	-1.703698	7.178662	-0.189108
N	3.340495	3.167755	1.148860	H	-3.087734	7.471850	1.867620



Zero-point correction= 0.329657 (Hartree/Particle)
 Thermal correction to Energy= 0.349534
 Thermal correction to Enthalpy= 0.350478
 Thermal correction to Gibbs Free Energy= 0.279080
 Sum of electronic and zero-point Energies= -825.860877
 Sum of electronic and thermal Energies= -825.841000
 Sum of electronic and thermal Enthalpies= -825.840056
 Sum of electronic and thermal Free Energies= -825.911454

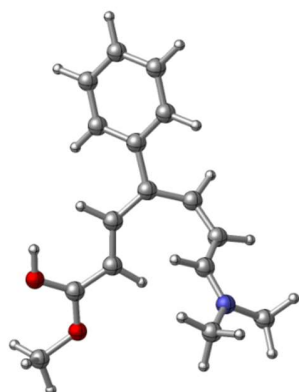
3a-OH-aii'

E(scf) = -826.172422162 a.u.

$\nu_{\min} = 33.33 \text{ cm}^{-1}$

C	-0.198834	4.045906	0.175964	N	1.796037	1.874445	2.393536
C	-1.600991	3.874786	0.415434	C	3.098936	1.752120	1.735781
C	-2.233391	2.650286	0.671641	H	3.666953	0.945002	2.212432
H	0.049414	4.854900	-0.521777	H	2.967204	1.515939	0.670880
H	-3.307884	2.752181	0.866713	H	3.666296	2.691528	1.830157
C	-1.742310	1.334357	0.604799	C	1.642913	1.209115	3.686517
H	-0.709626	1.122694	0.329902	H	1.810706	0.127821	3.569828
C	0.896963	3.377823	0.705933	H	2.382451	1.606211	4.399183
C	-2.524045	0.209085	0.828533	H	0.633837	1.380609	4.080254
O	-3.789811	0.182961	1.217552	C	-2.446315	5.092529	0.254710
O	-1.982958	-0.977522	0.654189	C	-3.726976	5.043295	-0.334602
C	0.822121	2.593100	1.873640	C	-1.968419	6.346247	0.689087
H	-0.115517	2.588503	2.435866	C	-4.501662	6.197208	-0.469822
H	1.873021	3.571038	0.257211	H	-4.112415	4.096248	-0.719922
C	-2.756145	-2.166521	0.894340	C	-2.739272	7.502610	0.544556
H	-3.098677	-2.200464	1.938605	H	-0.989007	6.411975	1.169988
H	-3.623879	-2.205540	0.220420	C	-4.011560	7.433050	-0.032100
H	-2.077951	-3.001923	0.688871	H	-5.488752	6.133112	-0.934756

H	-2.347555	8.460900	0.895013	H	-4.616957	8.336001	-0.142536
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Zero-point correction=	0.329684 (Hartree/Particle)
Thermal correction to Energy=	0.349435
Thermal correction to Enthalpy=	0.350379
Thermal correction to Gibbs Free Energy=	0.279735
Sum of electronic and zero-point Energies=	-825.842738
Sum of electronic and thermal Energies=	-825.822987
Sum of electronic and thermal Enthalpies=	-825.822043
Sum of electronic and thermal Free Energies=	-825.892687

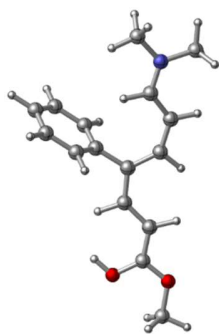
3a-OH-int'

E(scf) = -826.179621676 a.u.

$\nu_{\min} = 23.47 \text{ cm}^{-1}$

C	-0.214486	1.905558	0.879927	C	-4.446254	-2.707820	-1.275786
C	-1.538248	2.363624	0.678244	H	-5.299492	-2.694822	-0.582927
C	-2.537570	1.495119	0.210803	H	-4.763785	-2.338410	-2.261260
H	-0.017088	0.891226	0.520369	H	-4.038960	-3.720979	-1.360718
H	-3.507112	1.986106	0.058935	N	1.992990	4.311948	2.667695
C	-2.468143	0.122357	-0.064265	C	3.317096	3.694342	2.592290
H	-1.558403	-0.454724	0.100113	H	3.323525	2.729078	3.121849
C	0.906643	2.510494	1.455622	H	3.604984	3.527279	1.543499
C	-3.540444	-0.620673	-0.552220	H	4.052003	4.359113	3.059857
O	-4.751589	-0.174756	-0.836138	C	1.890501	5.585973	3.375939
O	-3.367726	-1.904309	-0.761168	H	2.205375	5.461133	4.423814
C	0.926679	3.744875	2.128097	H	2.543375	6.333498	2.899139
H	-0.001011	4.303108	2.253599	H	0.854589	5.946059	3.350634
H	1.833263	1.936655	1.405103	C	-1.932953	3.785550	0.930660

C	-2.784506	4.120214	1.996527	H	-0.791754	4.563044	-0.735060
C	-1.452980	4.813840	0.098285	C	-2.641727	6.468952	1.411623
C	-3.135835	5.453820	2.236501	H	-3.794694	5.699099	3.073259
H	-3.161348	3.329311	2.650158	H	-1.421358	6.932351	-0.316524
C	-1.802295	6.144486	0.338166	H	-2.912749	7.510586	1.600588



Zero-point correction=	0.329804 (Hartree/Particle)
Thermal correction to Energy=	0.349659
Thermal correction to Enthalpy=	0.350603
Thermal correction to Gibbs Free Energy=	0.279311
Sum of electronic and zero-point Energies=	-825.849818
Sum of electronic and thermal Energies=	-825.829962
Sum of electronic and thermal Enthalpies=	-825.829018
Sum of electronic and thermal Free Energies=	-825.900311

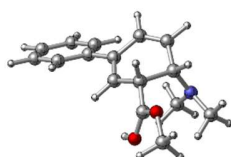
3a-OH-p1'

E(scf) = -826.155911126 a.u.

$\nu_{\min} = 43.13 \text{ cm}^{-1}$

C	-1.428226	4.500650	0.968406	H	-2.770742	5.492232	-0.349635
C	-1.170423	3.370435	1.878433	C	-5.728290	-0.270340	0.033311
C	-1.969548	2.278483	1.802739	H	-5.378387	-1.152151	0.583864
H	-1.812461	1.433524	2.479697	H	-6.556815	0.217737	0.563594
C	-2.997270	2.180393	0.712981	H	-6.007107	-0.522122	-0.993459
H	-2.510766	1.932863	-0.247309	N	-4.732008	4.091713	1.244354
C	-2.570684	4.613262	0.268041	C	-4.419968	4.342172	2.638296
C	-4.026781	1.147389	0.922633	H	-4.355500	3.414414	3.247406
O	-4.395442	0.715819	2.082665	H	-3.462681	4.870097	2.736254
O	-4.630020	0.683120	-0.099923	H	-5.205070	4.971065	3.085197
C	-3.699331	3.611982	0.378489	C	-6.079606	3.604522	1.008597
H	-4.146347	3.470112	-0.615193	H	-6.283163	2.614994	1.472396

H	-6.811607	4.306795	1.437473	H	0.496368	1.379820	2.741873
H	-6.276626	3.525202	-0.070458	C	1.259839	4.798962	4.422107
H	-0.667621	5.280824	0.891276	H	-0.334574	5.596016	3.213092
C	-0.064866	3.470536	2.863137	C	1.997589	3.665391	4.779364
C	0.690985	2.338911	3.227256	H	2.291228	1.547716	4.438821
C	0.242174	4.704400	3.469667	H	1.475613	5.763200	4.888811
C	1.710366	2.435442	4.176558	H	2.797723	3.741116	5.519692



Zero-point correction=	0.331189 (Hartree/Particle)
Thermal correction to Energy=	0.349514
Thermal correction to Enthalpy=	0.350458
Thermal correction to Gibbs Free Energy=	0.284743
Sum of electronic and zero-point Energies=	-825.824722
Sum of electronic and thermal Energies=	-825.806397
Sum of electronic and thermal Enthalpies=	-825.805453
Sum of electronic and thermal Free Energies=	-825.871168

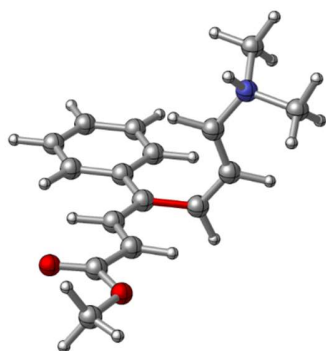
TS-3a-H-r

E(scf) = -826.125523135 a.u.

$\nu_{\min} = -132.02 \text{ cm}^{-1}$

C	-0.434502	2.333880	-0.429767	O	-3.250659	-1.753329	-1.368559
C	-1.821048	2.622315	0.015081	C	0.310504	1.403319	1.695879
C	-2.798828	1.619030	-0.160562	H	-0.640931	1.573625	2.201153
H	-0.161427	2.581064	-1.461922	H	1.522787	1.578758	-0.065358
H	-3.827967	1.823422	0.144799	C	-4.238748	-2.770528	-1.551110
C	-2.572075	0.367200	-0.692824	H	-4.684000	-3.061241	-0.587022
H	-1.584629	0.048491	-1.031590	H	-5.043150	-2.419299	-2.215743
C	0.541791	1.752701	0.382495	H	-3.720826	-3.625313	-2.002491
C	-3.673579	-0.596860	-0.821559	N	1.342709	0.854161	2.589285
O	-4.827881	-0.402902	-0.485093	C	2.461669	0.119061	1.909631

H	3.064663	-0.370560	2.683071	C	-1.071176	4.875133	0.779461
H	2.033627	-0.625269	1.228980	C	-3.659392	5.553321	1.576100
H	3.081150	0.834413	1.358598	H	-4.253825	3.614095	0.896561
C	1.865730	1.919089	3.526362	C	-1.319730	6.125422	1.340954
H	2.547281	1.449091	4.246360	H	-0.054499	4.621088	0.473657
H	2.390400	2.671361	2.926015	C	-2.614650	6.473856	1.744230
H	1.015039	2.374945	4.046085	H	-4.673767	5.816067	1.885894
C	-2.112197	3.926445	0.600178	H	-0.497771	6.834594	1.465390
C	-3.417489	4.303443	1.014925	H	-2.810348	7.454131	2.185062



Zero-point correction=	0.328153 (Hartree/Particle)
Thermal correction to Energy=	0.347297
Thermal correction to Enthalpy=	0.348241
Thermal correction to Gibbs Free Energy=	0.278984
Sum of electronic and zero-point Energies=	-825.797370
Sum of electronic and thermal Energies=	-825.778227
Sum of electronic and thermal Enthalpies=	-825.777282
Sum of electronic and thermal Free Energies=	-825.846539

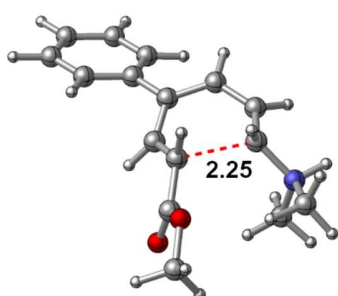
TS-3a-uu

E(scf) = -826.141145497 a.u.

$\nu_{\min} = -461.34 \text{ cm}^{-1}$

C	-1.475648	4.685812	1.460235	C	-3.733904	4.105369	0.541553
C	-1.053997	3.468102	2.053679	H	-3.623007	3.629552	-0.425361
C	-1.938927	2.379327	2.131220	H	-3.093857	6.025537	1.254038
H	-1.950017	1.787563	3.052562	C	-5.681033	-0.242253	0.578587
C	-2.904344	2.102290	1.159788	H	-5.331785	-1.132904	1.120843
H	-2.596550	2.112460	0.118067	H	-6.490983	0.230533	1.154140
C	-2.771869	4.994599	1.045469	H	-6.030843	-0.516069	-0.423161
C	-4.005231	1.156088	1.489633	N	-5.165238	4.489258	0.773012
O	-4.362270	0.878574	2.615246	C	-5.559350	4.290918	2.211412
O	-4.597113	0.680350	0.382787	H	-5.484443	3.223938	2.450983

H	-4.868503	4.859647	2.843873	C	0.708234	4.562024	3.526205
H	-6.586115	4.650326	2.347477	C	2.079858	2.133738	3.713201
C	-6.089182	3.775512	-0.166988	H	0.532713	1.333035	2.440489
H	-5.937323	2.697448	-0.044846	C	1.886047	4.479078	4.270845
H	-7.122749	4.050413	0.071615	H	0.168905	5.510731	3.492668
H	-5.844677	4.073126	-1.193362	C	2.577408	3.265790	4.366534
H	-0.815413	5.543925	1.609022	H	2.614689	1.183053	3.777662
C	0.196760	3.431712	2.857317	H	2.260593	5.365260	4.788973
C	0.902232	2.216218	2.966964	H	3.499404	3.203679	4.949693



Zero-point correction= 0.331492 (Hartree/Particle)
 Thermal correction to Energy= 0.349737
 Thermal correction to Enthalpy= 0.350681
 Thermal correction to Gibbs Free Energy= 0.284361
 Sum of electronic and zero-point Energies= -825.809654
 Sum of electronic and thermal Energies= -825.791409
 Sum of electronic and thermal Enthalpies= -825.790464
 Sum of electronic and thermal Free Energies= -825.856784

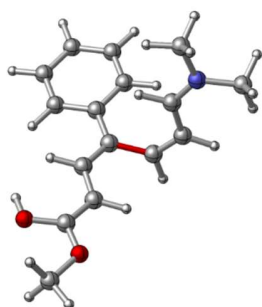
TS-3a-OH-r'

E(scf)=-826.160268552 a.u.

$\nu_{\min} = -51.81 \text{ cm}^{-1}$

C	-0.347471	3.008542	-0.402235	H	-0.286280	3.114006	2.204415
C	-1.724816	3.196185	0.125307	H	1.748686	2.803897	-0.160688
C	-2.500261	2.081484	0.298695	C	-3.314776	-2.716775	0.124653
H	-0.237521	2.907535	-1.490452	H	-3.710803	-2.815871	1.146397
H	-3.512549	2.249816	0.680925	H	-4.153965	-2.643502	-0.583497
C	-2.109069	0.726830	0.056135	H	-2.693258	-3.585918	-0.120900
H	-1.097380	0.494356	-0.278534	N	1.704127	3.047002	2.613996
C	0.788552	2.938155	0.337953	C	3.121097	2.965782	2.245784
C	-2.928876	-0.360272	0.230698	H	3.544050	2.042293	2.667382
O	-4.209502	-0.345227	0.612390	H	3.256548	2.970089	1.161470
O	-2.449206	-1.580747	0.015997	H	3.645690	3.827856	2.681586
C	0.714909	3.039058	1.767624	C	1.456436	3.137032	4.058321

H	1.888808	2.254398	4.551658	H	-4.313412	4.096056	0.452630
H	1.945848	4.039946	4.451424	C	-1.713704	6.961159	0.721439
H	0.379617	3.182378	4.255911	H	-0.211685	5.483922	0.323706
C	-2.190504	4.579987	0.380231	C	-3.071121	7.233862	0.904133
C	-3.562959	4.882910	0.546009	H	-5.060479	6.377639	0.935673
C	-1.279631	5.657747	0.461583	H	-0.978808	7.768258	0.779847
C	-3.992268	6.181809	0.811017	H	-3.411463	8.252056	1.106655



Zero-point correction=	0.328820 (Hartree/Particle)
Thermal correction to Energy=	0.348145
Thermal correction to Enthalpy=	0.349089
Thermal correction to Gibbs Free Energy=	0.279007
Sum of electronic and zero-point Energies=	-825.831449
Sum of electronic and thermal Energies=	-825.812123
Sum of electronic and thermal Enthalpies=	-825.811179
Sum of electronic and thermal Free Energies=	-825.881261

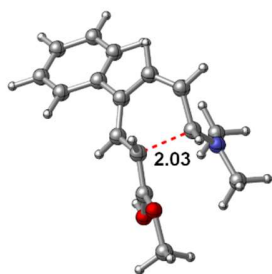
3a-OH-uu'

E(scf) = -826.149706076 a.u.

$\nu_{\min} = -307.35 \text{ cm}^{-1}$

C	-1.410479	4.391634	0.930068	H	-2.750047	5.513512	-0.268308
C	-1.131636	3.269447	1.840314	C	-5.733195	-0.222165	-0.101876
C	-1.896159	2.147435	1.769402	H	-5.464166	-1.159402	0.402954
H	-1.759256	1.360121	2.519653	H	-6.516898	0.299789	0.465379
C	-2.873745	1.954270	0.688554	H	-6.062293	-0.413579	-1.128000
H	-2.482058	1.992298	-0.334129	N	-4.752900	4.067847	1.341893
C	-2.593691	4.605233	0.323901	C	-4.435762	4.619765	2.653592
C	-3.922527	1.022625	0.829705	H	-4.479057	3.832294	3.426267
O	-4.379963	0.577554	1.978186	H	-3.433614	5.061558	2.653596
O	-4.568301	0.626326	-0.228130	H	-5.169617	5.397876	2.912693
C	-3.807749	3.740262	0.435456	C	-6.100542	3.527729	1.206745
H	-4.233226	3.441481	-0.527685	H	-6.245364	2.656703	1.869383

H	-6.839080	4.293838	1.487106	H	0.552248	1.341322	2.801637
H	-6.286268	3.224056	0.168204	C	1.215055	4.822256	4.393863
H	-0.620041	5.132773	0.787070	H	-0.365658	5.553442	3.128074
C	-0.052128	3.423053	2.846335	C	1.963268	3.713694	4.804225
C	0.716579	2.317714	3.263118	H	2.299352	1.591921	4.536638
C	0.220578	4.679886	3.423142	H	1.403538	5.804419	4.834460
C	1.710193	2.461113	4.233664	H	2.744473	3.826346	5.559910



Zero-point correction=	0.329782 (Hartree/Particle)
Thermal correction to Energy=	0.348140
Thermal correction to Enthalpy=	0.349084
Thermal correction to Gibbs Free Energy=	0.283185
Sum of electronic and zero-point Energies=	-825.819924
Sum of electronic and thermal Energies=	-825.801566
Sum of electronic and thermal Enthalpies=	-825.800622
Sum of electronic and thermal Free Energies=	-825.866521

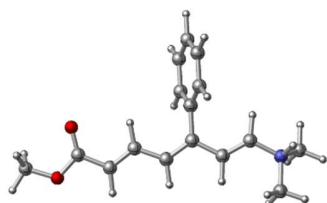
3b-H

E(scf) = -826.180724363 a.u.

$\nu_{\min} = 25.09 \text{ cm}^{-1}$

C	0.332391	2.414253	-0.693750	C	-1.953744	1.775272	0.088560
C	-1.024131	2.357082	-0.849714	H	-1.561597	1.300354	0.992724

C	-3.293738	1.777918	-0.091249	H	3.222451	4.502675	-4.800937
H	-3.759731	2.237459	-0.966659	C	3.855459	5.137328	-2.275290
C	1.120692	3.014896	-1.769242	H	4.526443	5.532677	-3.047337
C	-4.190919	1.152805	0.905834	H	3.049780	5.848175	-2.058170
O	-3.834174	0.605482	1.930011	H	4.418260	4.911599	-1.362189
O	-5.477618	1.265791	0.535794	H	-1.456083	2.773579	-1.766262
C	2.446320	3.211271	-1.719133	C	1.021804	1.920399	0.534011
H	3.068115	2.935532	-0.866986	C	0.771571	2.520792	1.780377
H	0.550208	3.324210	-2.647588	C	1.933015	0.850786	0.465166
C	-6.449521	0.699219	1.420302	C	1.414304	2.059456	2.932654
H	-6.282799	-0.382154	1.540687	H	0.070705	3.356634	1.841729
H	-6.397910	1.175074	2.411576	C	2.571439	0.388234	1.618814
H	-7.427704	0.883966	0.960698	H	2.131716	0.372066	-0.496851
N	3.228493	3.863692	-2.787437	C	2.314745	0.992102	2.854939
C	2.505437	4.094861	-4.079681	H	1.210280	2.536707	3.894222
H	2.106381	3.141101	-4.442062	H	3.269088	-0.450223	1.552703
H	1.697369	4.815494	-3.912164	H	2.815591	0.630422	3.756242



Zero-point correction=	0.332100 (Hartree/Particle)
Thermal correction to Energy=	0.351548
Thermal correction to Enthalpy=	0.352492
Thermal correction to Gibbs Free Energy=	0.281583
Sum of electronic and zero-point Energies=	-825.848624
Sum of electronic and thermal Energies=	-825.829177
Sum of electronic and thermal Enthalpies=	-825.828232
Sum of electronic and thermal Free Energies=	-825.899141

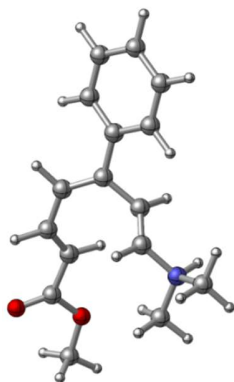
3b-H-aii

E(scf) = -826.172613092 a.u.

$\nu_{\min} = 25.06 \text{ cm}^{-1}$

C	-0.828043	4.762772	1.789883	C	-0.228275	3.544576	1.669800
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C	-0.810890	2.222600	1.869980	H	-5.281110	4.774830	-0.481637
H	-0.395412	1.414054	1.256814	H	-6.452164	5.315794	0.774038
C	-1.775681	1.887138	2.751162	C	-5.223559	3.104404	1.702011
H	-2.208397	2.614072	3.440203	H	-6.273336	3.205094	2.002291
C	-2.284545	4.900849	2.039713	H	-5.152960	2.574917	0.744264
C	-2.336810	0.521543	2.793905	H	-4.650961	2.569859	2.469510
O	-1.912756	-0.448900	2.202613	H	0.821240	3.536174	1.359809
O	-3.441407	0.492036	3.569733	C	-0.070726	6.032828	1.666950
C	-3.208730	4.412710	1.214946	C	1.294850	6.112801	2.011999
H	-2.990856	3.875785	0.289960	C	-0.712179	7.200841	1.206451
H	-2.586752	5.455822	2.937389	C	1.995218	7.311757	1.879475
C	-4.109535	-0.769679	3.683365	H	1.807156	5.235342	2.411916
H	-4.447113	-1.121293	2.696545	C	-0.009018	8.400440	1.074056
H	-3.437475	-1.525965	4.116094	H	-1.768208	7.166736	0.929226
H	-4.969286	-0.603190	4.343033	C	1.347608	8.460397	1.407800
N	-4.643497	4.484195	1.521273	H	3.051063	7.353754	2.157739
C	-5.394301	5.276968	0.486822	H	-0.523573	9.291626	0.706587
H	-4.966200	6.285082	0.445970	H	1.897486	9.399406	1.308788



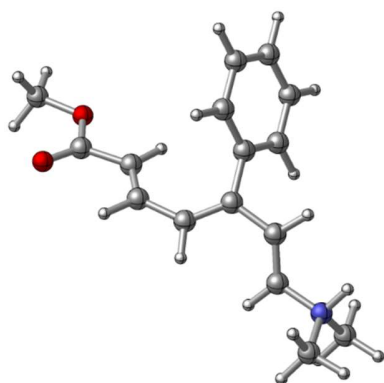
Zero-point correction= 0.331139 (Hartree/Particle)
 Thermal correction to Energy= 0.350753
 Thermal correction to Enthalpy= 0.351697
 Thermal correction to Gibbs Free Energy= 0.280886
 Sum of electronic and zero-point Energies= -825.841474
 Sum of electronic and thermal Energies= -825.821860
 Sum of electronic and thermal Enthalpies= -825.820916
 Sum of electronic and thermal Free Energies= -825.891728

3b-H-int

E(scf) = -826.171415585 a.u.

 $\nu_{\min} = 27.03 \text{ cm}^{-1}$

C	-2.279705	4.324355	1.223813	H	-5.098865	5.179150	-2.181811
C	-2.423652	2.983933	1.018054	H	-6.563217	4.588018	-1.317077
C	-1.708860	1.873475	1.633082	H	-6.547224	6.242074	-2.026630
H	-1.730018	0.929300	1.077227	C	-6.494214	6.481055	0.667532
C	-1.091226	1.848992	2.833321	H	-7.099440	7.228330	0.140197
H	-1.041882	2.719092	3.488892	H	-7.111482	5.616795	0.941123
C	-3.219592	5.272990	0.601853	H	-6.032435	6.917700	1.560330
C	-0.451495	0.605915	3.321594	H	-3.173217	2.675970	0.281944
O	-0.405020	-0.450762	2.724511	C	-1.184213	4.950652	2.017365
O	0.087976	0.792186	4.538540	C	0.163862	4.666829	1.732345
C	-4.522997	5.035112	0.414741	C	-1.484511	5.869515	3.037915
H	-5.047554	4.132146	0.730923	C	1.184966	5.271724	2.465862
H	-2.806460	6.247519	0.313717	H	0.405244	3.963819	0.932248
C	0.742739	-0.335753	5.127182	C	-0.460367	6.468426	3.778444
H	0.039341	-1.173327	5.251402	H	-2.528039	6.103791	3.264348
H	1.580878	-0.671539	4.497492	C	0.875953	6.169795	3.495427
H	1.111892	-0.001460	6.104026	H	2.227925	5.044063	2.232249
N	-5.398710	6.009565	-0.250507	H	-0.708402	7.170900	4.577874
C	-5.943329	5.463884	-1.543991	H	1.676877	6.639952	4.071217



Zero-point correction= 0.331591 (Hartree/Particle)
Thermal correction to Energy= 0.351162
Thermal correction to Enthalpy= 0.352106
Thermal correction to Gibbs Free Energy= 0.281454

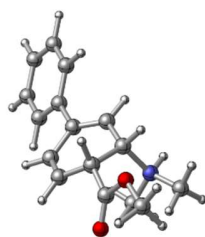
Sum of electronic and zero-point Energies= -825.839825
 Sum of electronic and thermal Energies= -825.820253
 Sum of electronic and thermal Enthalpies= -825.819309
 Sum of electronic and thermal Free Energies= -825.889962

3b-H-p1

E(scf) = -826.201947898 a.u.

$\nu_{\min} = 38.99 \text{ cm}^{-1}$

C	-1.548042	4.666207	1.249676	H	-4.812717	3.338393	2.973126
C	-1.474174	3.568962	2.231554	H	-3.879811	4.870573	2.818085
C	-2.253673	2.482116	2.116393	H	-5.671518	4.918474	2.934476
H	-2.203508	1.660590	2.833043	C	-6.221772	3.651138	0.652050
C	-3.158487	2.324973	0.924486	H	-6.345587	2.687795	1.155510
H	-2.531600	1.939060	0.097700	H	-7.031207	4.322572	0.962640
C	-2.578675	4.704902	0.366121	H	-6.234422	3.523573	-0.436073
C	-4.254370	1.286473	1.121287	H	-0.752482	3.640138	3.046515
O	-4.671984	0.920023	2.196000	C	-0.499488	5.718157	1.255942
O	-4.718091	0.857948	-0.052262	C	0.042067	6.191111	2.466890
C	-3.663605	3.665374	0.354208	C	-0.034793	6.276080	0.048920
H	-4.022057	3.496066	-0.668692	C	1.002935	7.205172	2.470091
H	-2.688454	5.539935	-0.329953	H	-0.306459	5.785793	3.419173
C	-5.774864	-0.117722	-0.024375	C	0.931274	7.283932	0.053668
H	-5.449070	-1.016701	0.517646	H	-0.415959	5.898287	-0.902416
H	-6.667545	0.294846	0.469061	C	1.451778	7.754433	1.264511
H	-5.993249	-0.355552	-1.071145	H	1.401995	7.568166	3.420323
N	-4.917831	4.265047	1.067412	H	1.286191	7.697559	-0.893439
C	-4.809153	4.353183	2.560591	H	2.209028	8.542176	1.267931



Zero-point correction= 0.335033 (Hartree/Particle)
 Thermal correction to Energy= 0.352931
 Thermal correction to Enthalpy= 0.353875
 Thermal correction to Gibbs Free Energy= 0.288798
 Sum of electronic and zero-point Energies= -825.866915

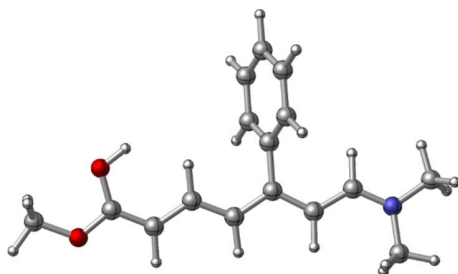
Sum of electronic and thermal Energies= -825.849017
 Sum of electronic and thermal Enthalpies= -825.848073
 Sum of electronic and thermal Free Energies= -825.913150

3b-OH'

E(scf) = -826.190169381 a.u.

$\nu_{\min} = 33.25 \text{ cm}^{-1}$

C	0.214746	2.655577	-0.721687	H	2.020445	3.601694	-4.392702
C	-1.188385	2.523146	-0.844714	H	1.724544	5.263367	-3.794829
C	-2.008696	1.849038	0.052053	H	3.283258	4.852471	-4.564959
H	-1.515011	1.379072	0.910624	C	4.468010	4.404497	-2.400960
C	-3.398435	1.724091	-0.075574	H	5.084160	3.876741	-3.145887
H	-3.920098	2.175365	-0.921130	H	4.648585	5.486636	-2.500342
C	0.946725	3.267251	-1.756567	H	4.768795	4.083817	-1.395830
C	-4.206634	1.038899	0.828824	H	-1.656935	2.968421	-1.728348
O	-3.812479	0.425281	1.931041	C	0.909073	2.143969	0.496661
O	-5.495711	0.975817	0.597886	C	0.630457	2.692726	1.761646
C	2.313364	3.550266	-1.670508	C	1.849445	1.102503	0.397750
H	2.846693	3.310814	-0.747254	C	1.282468	2.213080	2.900615
H	0.394864	3.560926	-2.651326	H	-0.093290	3.506548	1.846298
C	-6.364610	0.285043	1.515386	C	2.492098	0.617580	1.539964
H	-6.084936	-0.775842	1.583843	H	2.065848	0.665412	-0.579793
H	-6.315187	0.746227	2.511993	C	2.212115	1.172893	2.793114
H	-7.371163	0.388134	1.096156	H	1.064033	2.655066	3.875757
N	3.055029	4.108992	-2.618512	H	3.213530	-0.198104	1.449895
C	2.486193	4.476353	-3.913562	H	2.718195	0.795827	3.685127



Zero-point correction= 0.329828 (Hartree/Particle)
 Thermal correction to Energy= 0.349583

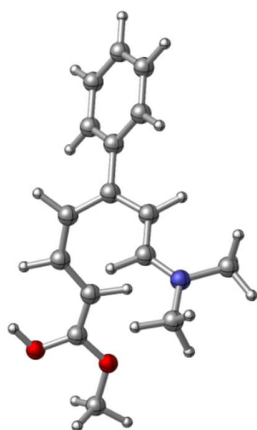
Thermal correction to Enthalpy=	0.350527
Thermal correction to Gibbs Free Energy=	0.279930
Sum of electronic and zero-point Energies=	-825.860341
Sum of electronic and thermal Energies=	-825.840586
Sum of electronic and thermal Enthalpies=	-825.839642
Sum of electronic and thermal Free Energies=	-825.910240

3b-OH-aii'

E(scf) = -826.177479145 a.u.

$\nu_{\min} = 29.15 \text{ cm}^{-1}$

C	-0.995445	4.896648	1.327035	H	-4.684618	5.413233	3.055454
C	-0.378009	3.615300	1.139893	H	-5.176639	6.241907	1.544905
C	-0.704090	2.386430	1.701285	H	-6.270028	5.054728	2.312823
H	-0.036539	1.579253	1.371669	C	-5.543223	3.226330	0.743296
C	-1.660814	2.046053	2.681006	H	-6.117191	2.734967	1.543728
H	-2.323957	2.795533	3.111047	H	-6.248322	3.724912	0.059699
C	-2.375052	5.095031	1.503773	H	-4.978131	2.468802	0.186590
C	-1.810310	0.772137	3.205912	H	0.547526	3.624880	0.558467
O	-1.159152	-0.323906	2.843365	C	-0.109833	6.085781	1.315844
O	-2.694077	0.585260	4.164521	C	1.210819	6.001056	1.805401
C	-3.326588	4.147439	1.101919	C	-0.563102	7.327173	0.820291
H	-2.988405	3.275641	0.535830	C	2.044819	7.119724	1.807332
H	-2.715506	6.058171	1.885025	H	1.573986	5.055994	2.214295
C	-2.887832	-0.725521	4.722694	C	0.274860	8.442316	0.815383
H	-3.216067	-1.432300	3.946949	H	-1.569700	7.409650	0.405230
H	-1.959343	-1.091176	5.184288	C	1.580362	8.343229	1.311272
H	-3.667850	-0.606772	5.482793	H	3.060075	7.038378	2.202697
N	-4.628165	4.208363	1.320719	H	-0.088778	9.391753	0.415321
C	-5.220971	5.293143	2.103242	H	2.235104	9.218081	1.309284



Zero-point correction=	0.329980 (Hartree/Particle)
Thermal correction to Energy=	0.349619
Thermal correction to Enthalpy=	0.350563
Thermal correction to Gibbs Free Energy=	0.280402
Sum of electronic and zero-point Energies=	-825.847499
Sum of electronic and thermal Energies=	-825.827860
Sum of electronic and thermal Enthalpies=	-825.826916
Sum of electronic and thermal Free Energies=	-825.897077

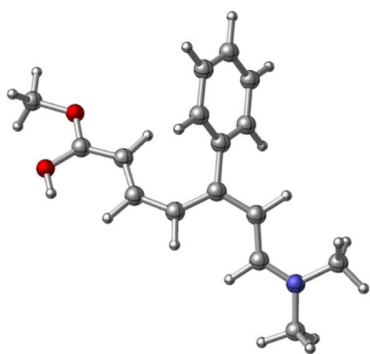
3b-OH-int'

E(scf) = -826.179928102 a.u.

$\nu_{\min} = 23.16 \text{ cm}^{-1}$

C	-2.231001	4.304843	1.258038	H	-0.594605	3.182484	3.575930
C	-2.190905	2.883299	1.183787	C	-3.261578	5.077825	0.687847
C	-1.486307	1.984971	1.982679	C	-0.080373	1.169741	3.833185
H	-1.617820	0.942197	1.664807	O	-0.039670	-0.110980	3.502955
C	-0.714971	2.193702	3.138848	O	0.560010	1.467226	4.941002

C	-4.462630	4.549008	0.198376	H	-6.848024	4.740827	-1.864967
H	-4.663491	3.480190	0.307943	H	-6.650054	3.528421	-0.561455
H	-3.112668	6.157510	0.660611	H	-2.826506	2.415251	0.429207
C	1.248651	0.441128	5.678097	C	-1.125470	5.064888	1.901511
H	0.541174	-0.326569	6.022605	C	0.212211	4.813019	1.541442
H	2.025400	-0.025356	5.055472	C	-1.398488	6.068770	2.848534
H	1.702308	0.952092	6.534244	C	1.249908	5.544259	2.118787
N	-5.432128	5.238162	-0.384799	H	0.429627	4.039018	0.802474
C	-5.313853	6.677400	-0.615364	C	-0.355738	6.786715	3.440461
H	-5.290183	7.222972	0.341379	H	-2.432744	6.267966	3.138526
H	-4.394395	6.902005	-1.176097	C	0.969626	6.528003	3.075736
H	-6.176591	7.020924	-1.197241	H	2.282972	5.346158	1.823115
C	-6.684224	4.601775	-0.785119	H	-0.579850	7.551007	4.188438
H	-7.527965	5.054961	-0.241064	H	1.784324	7.093640	3.534401



Zero-point correction=	0.329591 (Hartree/Particle)
Thermal correction to Energy=	0.349466
Thermal correction to Enthalpy=	0.350410
Thermal correction to Gibbs Free Energy=	0.278964
Sum of electronic and zero-point Energies=	-825.850337
Sum of electronic and thermal Energies=	-825.830462
Sum of electronic and thermal Enthalpies=	-825.829518
Sum of electronic and thermal Free Energies=	-825.900964

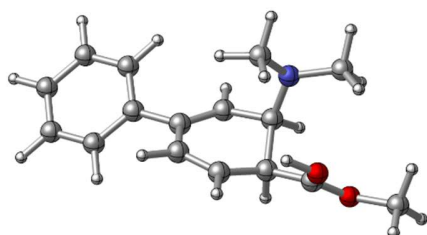
3b-OH-p1'

E(scf) = -826.154802508a.u.

$\nu_{\min} = 32.34 \text{ cm}^{-1}$

C	-1.675113	4.305861	0.236390	H	-1.312150	0.930306	-0.444398
C	-1.084074	3.019681	-0.171756	C	-3.161018	1.871074	0.457299
C	-1.779910	1.869941	-0.135268	H	-3.092169	1.892343	1.559134

C	-3.016600	4.388530	0.406049	C	-5.914798	2.813795	-1.315864
C	-3.986661	0.696111	0.127010	H	-5.900658	1.730039	-1.562719
O	-3.846874	-0.012640	-0.943558	H	-6.513858	2.950211	-0.403713
O	-4.931998	0.382248	0.922102	H	-6.438350	3.315442	-2.144973
C	-3.969225	3.245461	0.134652	H	-0.054035	3.015372	-0.534420
H	-4.769677	3.270520	0.886700	C	-0.780471	5.481220	0.408604
H	-3.494114	5.335921	0.665490	C	-1.198660	6.775026	0.042383
C	-5.846350	-0.715706	0.617825	C	0.509589	5.323853	0.950393
H	-6.391093	-0.477925	-0.305442	C	-0.359453	7.876172	0.224491
H	-5.271000	-1.642655	0.503125	H	-2.182184	6.916592	-0.411387
H	-6.520850	-0.765185	1.476807	C	1.348031	6.426404	1.135281
N	-4.593287	3.390710	-1.145953	H	0.856367	4.332182	1.251199
C	-3.767505	3.365227	-2.336865	C	0.916833	7.706800	0.773423
H	-3.447791	2.340676	-2.628411	H	-0.700068	8.870921	-0.073567
H	-4.329401	3.783204	-3.186149	H	2.342024	6.283835	1.566510
H	-2.861379	3.968618	-2.196395	H	1.574219	8.568475	0.912967



Zero-point correction=	0.331013 (Hartree/Particle)
Thermal correction to Energy=	0.349411
Thermal correction to Enthalpy=	0.350355
Thermal correction to Gibbs Free Energy=	0.284292
Sum of electronic and zero-point Energies=	-825.823790
Sum of electronic and thermal Energies=	-825.805392
Sum of electronic and thermal Enthalpies=	-825.804447
Sum of electronic and thermal Free Energies=	-825.870511

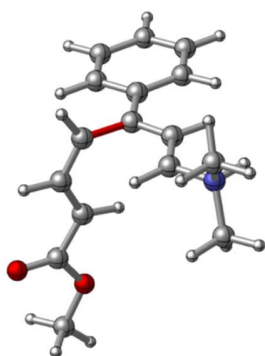
TS-3b-H-r

E(scf) = -826.128660070 a.u.

$\nu_{\min} = -129.7 \text{ cm}^{-1}$

C	-1.549431	4.874941	1.103530	C	-1.223326	3.591111	0.433038
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C	-1.220695	2.359343	1.069616	H	-5.932033	4.317911	-1.246367
H	-0.978402	1.469015	0.480852	H	-6.910215	5.695606	-0.625387
C	-1.510221	2.164218	2.419655	C	-6.187470	4.175685	1.482948
H	-1.758505	3.001762	3.075296	H	-7.193547	4.609737	1.534896
C	-2.906212	5.296204	1.102523	H	-6.224421	3.186671	1.010851
C	-1.490240	0.819209	3.007516	H	-5.743993	4.103942	2.482543
O	-1.235006	-0.208331	2.405926	H	-0.991403	3.627252	-0.638448
O	-1.795551	0.851900	4.318591	C	-0.486612	5.651786	1.721137
C	-3.937692	4.574037	0.576020	C	0.846939	5.161124	1.707404
H	-3.847549	3.597747	0.099034	C	-0.714571	6.903277	2.356086
H	-3.148296	6.256981	1.565725	C	1.887066	5.877065	2.293641
C	-1.803933	-0.404413	5.001921	H	1.059456	4.202015	1.232187
H	-2.541687	-1.087977	4.553978	C	0.329183	7.613322	2.939986
H	-0.812381	-0.880613	4.955517	H	-1.716840	7.331325	2.397311
H	-2.071408	-0.186612	6.042822	C	1.637214	7.107516	2.914496
N	-5.316550	5.070924	0.640757	H	2.901806	5.472863	2.267722
C	-5.898393	5.285519	-0.731274	H	0.123867	8.572302	3.421726
H	-5.252879	5.984097	-1.275434	H	2.453257	7.668931	3.375272



Zero-point correction=	0.327867 (Hartree/Particle)
Thermal correction to Energy=	0.347094
Thermal correction to Enthalpy=	0.348038
Thermal correction to Gibbs Free Energy=	0.278394
Sum of electronic and zero-point Energies=	-825.800793
Sum of electronic and thermal Energies=	-825.781566
Sum of electronic and thermal Enthalpies=	-825.780622
Sum of electronic and thermal Free Energies=	-825.850266

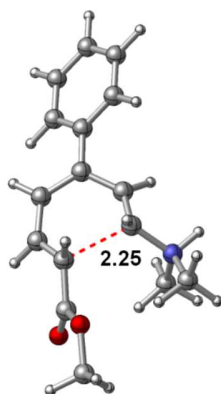
TS-3b-H-uu

E(scf) = -826.140727266 a.u.

$\nu_{\min} = -464.38 \text{ cm}^{-1}$

C	-1.353401	4.564919	1.216503	C	-1.040355	3.291752	1.756961
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C	-1.943536	2.248399	1.914730	H	-4.716652	4.940939	2.713834
H	-1.861837	1.631196	2.817001	H	-6.454168	4.777667	2.275141
C	-3.019076	2.001600	1.045274	C	-6.068609	3.773385	-0.209413
H	-2.807227	1.940590	-0.017788	H	-5.959078	2.696960	-0.038446
C	-2.679872	4.911489	0.882976	H	-7.082025	4.105109	0.043294
C	-4.124844	1.124751	1.515251	H	-5.842069	4.012023	-1.255348
O	-4.387671	0.910368	2.680380	H	-0.101473	3.226835	2.312665
O	-4.839454	0.632379	0.489586	C	-0.366005	5.675056	1.307745
C	-3.679381	4.059572	0.403441	C	0.600903	5.755842	2.329982
H	-3.607284	3.587530	-0.569198	C	-0.397057	6.696380	0.336858
H	-2.977803	5.928005	1.174238	C	1.504145	6.818819	2.374937
C	-5.940719	-0.226048	0.826572	H	0.633795	5.000613	3.117411
H	-5.581998	-1.112436	1.369755	C	0.508377	7.759190	0.381918
H	-6.667946	0.307721	1.456582	H	-1.123698	6.640388	-0.477268
H	-6.398985	-0.519466	-0.124658	C	1.463135	7.823859	1.401228
N	-5.090750	4.493171	0.670013	H	2.239215	6.867928	3.181904
C	-5.446280	4.372862	2.126156	H	0.471940	8.534678	-0.387023
H	-5.404860	3.315544	2.410808	H	2.173014	8.653711	1.438391



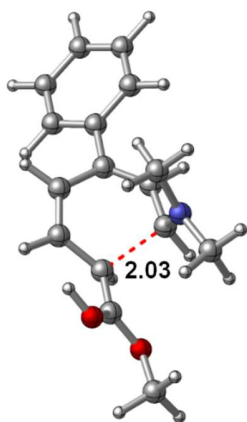
Zero-point correction=	0.331649 (Hartree/Particle)
Thermal correction to Energy=	0.349785
Thermal correction to Enthalpy=	0.350730
Thermal correction to Gibbs Free Energy=	0.284833
Sum of electronic and zero-point Energies=	-825.809078
Sum of electronic and thermal Energies=	-825.790942
Sum of electronic and thermal Enthalpies=	-825.789998
Sum of electronic and thermal Free Energies=	-825.855894

TS-3b-OH-dd'

E(scf) = -826.148431900 a.u.

 $\nu_{\min} = -318.87 \text{ cm}^{-1}$

C	-1.699789	4.302640	0.139861	H	-3.569880	2.688138	-2.996599
C	-1.091762	3.030920	-0.283235	H	-4.520623	4.188121	-3.188866
C	-1.721128	1.843961	-0.172074	H	-2.988131	4.216815	-2.269526
H	-1.241709	0.945121	-0.577580	C	-5.885780	2.629528	-1.472174
C	-3.013648	1.734280	0.527101	H	-5.718495	1.619665	-1.885053
H	-3.024769	2.060323	1.572894	H	-6.424133	2.543579	-0.519245
C	-3.046778	4.425905	0.244539	H	-6.514664	3.186728	-2.182902
C	-3.872497	0.644535	0.289048	H	-0.098786	3.074541	-0.736382
O	-3.844009	-0.112661	-0.785347	C	-0.798194	5.460155	0.388088
O	-4.838894	0.399626	1.126169	C	-1.176965	6.773992	0.051749
C	-4.067117	3.375099	-0.046140	C	0.465428	5.256840	0.975006
H	-4.806163	3.242002	0.750120	C	-0.325678	7.850547	0.308575
H	-3.491307	5.387725	0.519597	H	-2.136719	6.952937	-0.438230
C	-5.811016	-0.632992	0.841989	C	1.315084	6.334898	1.235914
H	-6.361025	-0.387536	-0.077556	H	0.779911	4.246853	1.248919
H	-5.309307	-1.603526	0.732178	C	0.922582	7.635737	0.904164
H	-6.484936	-0.639175	1.704376	H	-0.634326	8.861917	0.032691
N	-4.622396	3.330175	-1.276274	H	2.287533	6.157135	1.701657
C	-3.879693	3.622203	-2.495912	H	1.589170	8.478597	1.102487



Zero-point correction=

0.329477 (Hartree/Particle)

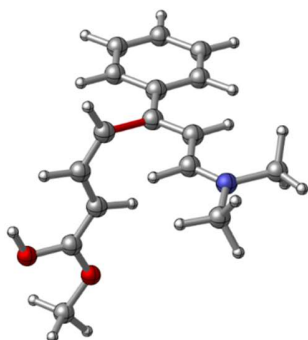
Thermal correction to Energy=	0.347983
Thermal correction to Enthalpy=	0.348927
Thermal correction to Gibbs Free Energy=	0.282336
Sum of electronic and zero-point Energies=	-825.818955
Sum of electronic and thermal Energies=	-825.800449
Sum of electronic and thermal Enthalpies=	-825.799505
Sum of electronic and thermal Free Energies=	-825.866096

TS-3b-OH-r'

E(scf) = -826.166183776 a.u.

$\nu_{\min} = -48.47 \text{ cm}^{-1}$

C	-1.487231	4.778150	1.005915	H	-5.438345	6.019048	1.956327
C	-1.075725	3.433971	0.512495	H	-5.224478	6.582941	0.266508
C	-0.974126	2.337195	1.302535	H	-6.744654	5.784489	0.760026
H	-0.650427	1.417800	0.798498	C	-6.073571	3.462968	0.119935
C	-1.261350	2.273514	2.709762	H	-6.789717	3.283259	0.935849
H	-1.620222	3.162553	3.230740	H	-6.624926	3.812860	-0.765682
C	-2.819243	5.141745	0.989869	H	-5.550812	2.529389	-0.119114
C	-1.126461	1.151760	3.481685	H	-0.833209	3.362867	-0.552358
O	-0.685717	-0.048031	3.084143	C	-0.438547	5.693337	1.487686
O	-1.457378	1.196385	4.770407	C	0.916136	5.292528	1.431134
C	-3.826133	4.231475	0.579425	C	-0.729606	6.973933	2.018203
H	-3.521421	3.224170	0.282510	C	1.934678	6.132783	1.878887
H	-3.118295	6.138153	1.309960	H	1.162357	4.308418	1.031120
C	-1.257002	0.045437	5.597101	C	0.288203	7.810003	2.465963
H	-1.860293	-0.805449	5.246308	H	-1.759117	7.324916	2.093707
H	-0.196576	-0.248535	5.618383	C	1.625523	7.394179	2.397278
H	-1.581426	0.342677	6.601501	H	2.974038	5.801457	1.823846
N	-5.111212	4.486161	0.533226	H	0.040889	8.792398	2.874426
C	-5.658749	5.797886	0.901797	H	2.422190	8.053593	2.749986



Zero-point correction= 0.328793 (Hartree/Particle)
 Thermal correction to Energy= 0.348045
 Thermal correction to Enthalpy= 0.348989
 Thermal correction to Gibbs Free Energy= 0.279018
 Sum of electronic and zero-point Energies= -825.837391
 Sum of electronic and thermal Energies= -825.818139
 Sum of electronic and thermal Enthalpies= -825.817194
 Sum of electronic and thermal Free Energies= -825.887166

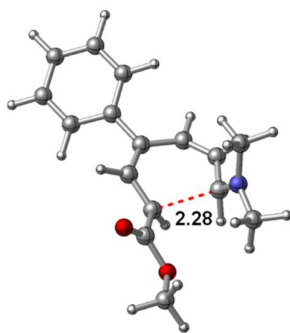
TS-3a-dd

E(scf) = -825.722679153 a.u.

$\nu_{\text{min}} = -271.06 \text{ cm}^{-1}$

C	-1.547054	4.106997	0.269649	H	-3.135298	5.365426	-0.292144
C	-0.823768	2.863735	0.199963	C	-5.792044	-0.612710	0.510099
C	-1.527881	1.668159	0.107577	H	-6.127548	-0.472052	-0.530238
H	-0.931139	5.009511	0.331151	H	-5.354365	-1.619034	0.598963
H	-1.080183	0.814194	-0.414938	H	-6.644026	-0.510704	1.194103
C	-2.850816	1.548967	0.581097	N	-4.773633	3.394766	-1.173988
H	-3.075396	1.991090	1.550823	C	-4.291287	3.794043	-2.486307
C	-2.880299	4.344852	0.022586	H	-4.465525	2.982333	-3.213256
C	-3.693194	0.431215	0.170332	H	-4.817342	4.694787	-2.845951
O	-3.460844	-0.360195	-0.728004	H	-3.215981	4.008468	-2.442312
O	-4.852664	0.392207	0.883719	C	-6.099912	2.798925	-1.142756
C	-3.988156	3.407018	-0.079620	H	-6.852846	3.511498	-1.519268
H	-4.508882	3.093769	0.821668	H	-6.134182	1.897497	-1.779443

H	-6.360119	2.511018	-0.116774	C	2.700809	3.927304	-0.825118
C	0.646584	2.880512	-0.001007	H	0.746895	4.801668	-1.011317
C	1.431007	1.788002	0.430165	C	3.458695	2.831002	-0.397132
C	1.317247	3.949686	-0.635024	H	3.391518	0.898786	0.576597
C	2.813113	1.759016	0.228637	H	3.189475	4.768541	-1.324304
H	0.946812	0.959418	0.952481	H	4.540994	2.813845	-0.548329



Zero-point correction=	0.315739 (Hartree/Particle)
Thermal correction to Energy=	0.334345
Thermal correction to Enthalpy=	0.335290
Thermal correction to Gibbs Free Energy=	0.267966
Sum of electronic and zero-point Energies=	-825.406940
Sum of electronic and thermal Energies=	-825.388334
Sum of electronic and thermal Enthalpies=	-825.387389
Sum of electronic and thermal Free Energies=	-825.454713

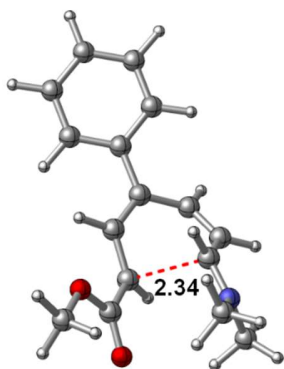
TS-3a-du

E(scf) = -825.712056002 a.u.

$\nu_{\min} = -560.69 \text{ cm}^{-1}$

C	-1.825050	4.186135	0.848739	H	-1.664171	0.982769	-0.401062
C	-1.251318	2.961139	0.268977	C	-3.336650	1.678047	0.778941
C	-2.038841	1.825142	0.191413	H	-3.558946	2.170960	1.726443
H	-1.152864	4.869300	1.379900	C	-3.132471	4.527591	0.765824

C	-4.316408	0.720803	0.379879	C	-6.253746	3.140284	-0.901967
O	-5.422861	0.559859	0.905017	H	-6.667735	2.201740	-0.507673
O	-3.966396	0.010665	-0.743264	H	-7.073152	3.834686	-1.142405
C	-4.071772	3.738376	-0.053605	H	-5.679950	2.925772	-1.811718
H	-3.722556	3.443866	-1.049290	C	0.135574	2.995644	-0.228194
H	-3.508344	5.431781	1.249486	C	0.921841	1.823424	-0.336370
C	-4.936512	-0.897438	-1.243924	C	0.739064	4.212486	-0.626010
H	-5.234683	-1.635257	-0.481839	C	2.223736	1.863951	-0.837280
H	-5.845186	-0.370380	-1.580875	H	0.513007	0.868716	0.001940
H	-4.472627	-1.410673	-2.097135	C	2.047554	4.253367	-1.112933
N	-5.381921	3.748677	0.104032	H	0.164383	5.140826	-0.577723
C	-6.006217	3.980550	1.402850	C	2.800415	3.079282	-1.227619
H	-6.981305	4.466787	1.261530	H	2.801817	0.938065	-0.906024
H	-6.150648	3.003214	1.893068	H	2.479054	5.211748	-1.415349
H	-5.371885	4.609845	2.036886	H	3.823955	3.110800	-1.609348



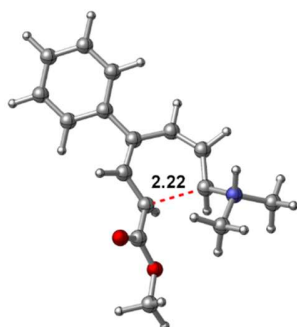
Zero-point correction=	0.315493 (Hartree/Particle)
Thermal correction to Energy=	0.334036
Thermal correction to Enthalpy=	0.334980
Thermal correction to Gibbs Free Energy=	0.268160
Sum of electronic and zero-point Energies=	-825.396563
Sum of electronic and thermal Energies=	-825.378020
Sum of electronic and thermal Enthalpies=	-825.377076
Sum of electronic and thermal Free Energies=	-825.443896

TS-3a-H-dd

E(scf) = -826.140311565 a.u.

ν_{\min} = -442.01 cm^{-1}

C	-1.516028	4.084252	0.318859	C	-5.450945	2.459764	-1.862617
C	-0.767430	2.890849	0.132568	H	-5.909751	1.813804	-1.106395
C	-1.421780	1.714408	-0.252648	H	-6.195533	2.765484	-2.606984
H	-0.934600	4.994690	0.484253	H	-4.615878	1.942130	-2.347174
H	-0.921446	1.020291	-0.934918	C	-6.036732	4.520246	-0.603020
C	-2.747952	1.458518	0.111420	H	-6.726816	4.796712	-1.409735
H	-3.022356	1.662803	1.143611	H	-6.557814	3.922556	0.154574
C	-2.846245	4.291098	-0.041220	H	-5.603821	5.417553	-0.146231
C	-3.469700	0.316372	-0.513866	C	0.717014	2.949379	0.080468
O	-3.133209	-0.243257	-1.534784	C	1.462473	1.817069	0.466870
O	-4.574470	0.003851	0.181177	C	1.417482	4.093184	-0.352381
C	-3.887717	3.344593	-0.147054	C	2.858328	1.828559	0.426720
H	-4.393237	2.914357	0.712410	H	0.939470	0.926945	0.824404
H	-3.061125	5.301441	-0.419815	C	2.813060	4.104250	-0.390761
C	-5.360364	-1.089933	-0.315527	H	0.870769	4.975113	-0.692245
H	-5.723451	-0.876298	-1.332334	C	3.539212	2.973193	-0.000730
H	-4.761833	-2.012235	-0.339799	H	3.416249	0.942183	0.738340
H	-6.202991	-1.198140	0.376706	H	3.336498	4.998396	-0.738033
N	-4.925172	3.687030	-1.178886	H	4.631431	2.984171	-0.031491



Zero-point correction=	0.331674 (Hartree/Particle)
Thermal correction to Energy=	0.349856
Thermal correction to Enthalpy=	0.350800
Thermal correction to Gibbs Free Energy=	0.284574
Sum of electronic and zero-point Energies=	-825.808637
Sum of electronic and thermal Energies=	-825.790456
Sum of electronic and thermal Enthalpies=	-825.789511
Sum of electronic and thermal Free Energies=	-825.855738

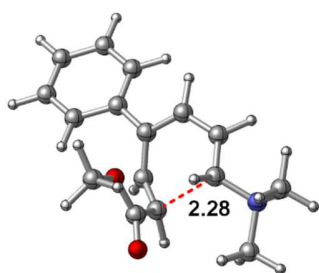
TS-3a-H-du

E(scf) = -826.134641835 a.u.

$\nu_{\min} = -452.13 \text{ cm}^{-1}$

C	-2.251304	3.857057	-0.942429	H	-1.731135	4.522908	-1.636005
C	-1.430928	2.949775	-0.226219	H	-1.202432	2.343545	1.796821
C	-1.904531	2.347457	0.954335	C	-3.215026	1.922469	1.221071

H	-3.504185	1.861826	2.275294	H	-5.414545	3.291625	2.595663
C	-3.557865	4.216293	-0.620375	C	-6.785416	4.198198	-0.396705
C	-3.872888	0.822429	0.459858	H	-7.116979	3.213035	-0.746137
O	-4.821014	0.197812	0.890590	H	-7.614193	4.730739	0.085765
O	-3.330648	0.605685	-0.743427	H	-6.389916	4.783847	-1.234150
C	-4.487431	3.365352	-0.010044	C	0.029935	2.897248	-0.498107
H	-4.791928	2.462373	-0.529165	C	0.712813	1.686270	-0.267108
H	-3.834345	5.265574	-0.792054	C	0.766506	4.000497	-0.973099
C	-3.914552	-0.434187	-1.542219	C	2.084925	1.579030	-0.505861
H	-3.823445	-1.405463	-1.034513	H	0.150977	0.815352	0.079070
H	-4.978508	-0.227063	-1.730211	C	2.137747	3.892680	-1.210630
H	-3.353752	-0.441328	-2.483768	H	0.275150	4.962591	-1.131500
N	-5.685731	3.995118	0.611841	C	2.802081	2.682173	-0.979415
C	-6.166560	3.213006	1.803851	H	2.593454	0.628322	-0.328206
H	-7.119663	3.637337	2.139612	H	2.693738	4.762541	-1.568761
H	-6.285571	2.163751	1.508156	H	3.875439	2.600804	-1.167370



Zero-point correction= 0.331309 (Hartree/Particle)
 Thermal correction to Energy= 0.349503
 Thermal correction to Enthalpy= 0.350447
 Thermal correction to Gibbs Free Energy= 0.284320
 Sum of electronic and zero-point Energies= -825.803333
 Sum of electronic and thermal Energies= -825.785139
 Sum of electronic and thermal Enthalpies= -825.784195
 Sum of electronic and thermal Free Energies= -825.850322

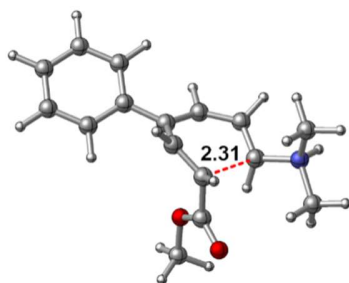
TS-3a-H-ud

E(scf) = -826.134517421 a.u.

$\nu_{\min} = -459.25 \text{ cm}^{-1}$

C	-1.334476	4.583610	-0.201692	C	-2.636249	4.948586	-0.547216
C	-0.814222	3.267200	-0.185375	C	-3.547089	1.825510	1.016000
C	-1.614786	2.178600	-0.593190	O	-4.614507	1.286580	1.226347
H	-0.593958	5.387788	-0.205431	O	-2.773713	2.335140	1.981812
H	-1.135787	1.485125	-1.295285	C	-3.759211	4.164524	-0.276412
C	-2.980453	1.986640	-0.352405	H	-3.979789	3.916320	0.754934
H	-3.516018	1.333948	-1.050926	H	-2.751804	5.870644	-1.132872

C	-3.252950	2.213489	3.329541	H	-6.331197	4.062554	0.587364
H	-4.225004	2.716376	3.441481	C	0.653681	3.050027	-0.093515
H	-3.364281	1.154291	3.603508	C	1.118913	1.855214	0.491628
H	-2.498239	2.694623	3.961961	C	1.603408	3.978809	-0.563601
N	-5.014124	4.436328	-1.036501	C	2.486901	1.597965	0.607988
C	-4.863924	4.129288	-2.499243	H	0.394885	1.135766	0.881719
H	-4.686363	3.052894	-2.601579	C	2.970131	3.720448	-0.447769
H	-5.785130	4.421726	-3.016745	H	1.277456	4.899213	-1.052295
H	-4.010381	4.688877	-2.897223	C	3.417411	2.530619	0.139306
C	-6.181962	3.706633	-0.438563	H	2.826257	0.669208	1.073015
H	-7.071240	3.911232	-1.044831	H	3.691269	4.448136	-0.827830
H	-5.952995	2.634756	-0.425874	H	4.488149	2.332028	0.229500



Zero-point correction=	0.331229 (Hartree/Particle)
Thermal correction to Energy=	0.349445
Thermal correction to Enthalpy=	0.350389
Thermal correction to Gibbs Free Energy=	0.284004
Sum of electronic and zero-point Energies=	-825.803288
Sum of electronic and thermal Energies=	-825.785072
Sum of electronic and thermal Enthalpies=	-825.784128
Sum of electronic and thermal Free Energies=	-825.850513

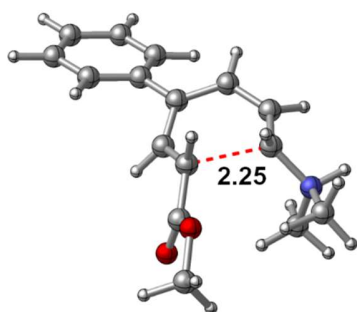
TS-3a-H-uu

E(scf) = -826.141145497 a.u.

$\nu_{\min} = -461.34 \text{ cm}^{-1}$

C	-1.475648	4.685812	1.460235	H	-3.623007	3.629552	-0.425361
C	-1.053997	3.468102	2.053679	H	-3.093857	6.025537	1.254038
C	-1.938927	2.379327	2.131220	C	-5.681033	-0.242253	0.578587
H	-1.950017	1.787563	3.052562	H	-5.331785	-1.132904	1.120843
C	-2.904344	2.102290	1.159788	H	-6.490983	0.230533	1.154140
H	-2.596550	2.112460	0.118067	H	-6.030843	-0.516069	-0.423161
C	-2.771869	4.994599	1.045469	N	-5.165238	4.489258	0.773012
C	-4.005231	1.156088	1.489633	C	-5.559350	4.290918	2.211412
O	-4.362270	0.878574	2.615246	H	-5.484443	3.223938	2.450983
O	-4.597113	0.680350	0.382787	H	-4.868503	4.859647	2.843873
C	-3.733904	4.105369	0.541553	H	-6.586115	4.650326	2.347477

C	-6.089182	3.775512	-0.166988	C	2.079858	2.133738	3.713201
H	-5.937323	2.697448	-0.044846	H	0.532713	1.333035	2.440489
H	-7.122749	4.050413	0.071615	C	1.886047	4.479078	4.270845
H	-5.844677	4.073126	-1.193362	H	0.168905	5.510731	3.492668
H	-0.815413	5.543925	1.609022	C	2.577408	3.265790	4.366534
C	0.196760	3.431712	2.857317	H	2.614689	1.183053	3.777662
C	0.902232	2.216218	2.966964	H	2.260593	5.365260	4.788973
C	0.708234	4.562024	3.526205	H	3.499404	3.203679	4.949693



Zero-point correction=	0.331492 (Hartree/Particle)
Thermal correction to Energy=	0.349737
Thermal correction to Enthalpy=	0.350681
Thermal correction to Gibbs Free Energy=	0.284361
Sum of electronic and zero-point Energies=	-825.809654
Sum of electronic and thermal Energies=	-825.791409
Sum of electronic and thermal Enthalpies=	-825.790464
Sum of electronic and thermal Free Energies=	-825.856784

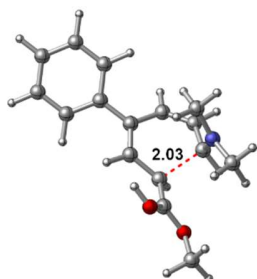
TS-3a-OH-dd'

E(scf) = -826.149667240 a.u.

$\nu_{\min} = -310.59 \text{ cm}^{-1}$

C	-1.662240	4.069067	0.722936	H	-6.354432	-0.394191	-0.420138
C	-0.981974	2.830133	0.313241	H	-5.454925	-1.681965	0.458950
C	-1.690788	1.671685	0.249872	H	-6.729256	-0.730326	1.312123
H	-1.037712	4.898589	1.064028	N	-4.385559	3.341465	-1.148271
H	-1.213460	0.776162	-0.164184	C	-3.468327	3.660805	-2.235829
C	-3.069096	1.587754	0.753893	H	-3.153339	2.741143	-2.759104
H	-3.220507	1.856871	1.805213	H	-3.972292	4.315669	-2.962806
C	-2.990218	4.273132	0.633549	H	-2.579515	4.172677	-1.851977
C	-3.917945	0.542153	0.336730	C	-5.637042	2.715813	-1.558137
O	-3.761082	-0.153767	-0.766506	H	-6.134838	3.340354	-2.315206
O	-4.993530	0.282630	1.021162	H	-5.455209	1.722114	-2.003276
C	-4.001512	3.286337	0.144693	H	-6.308423	2.607365	-0.696344
H	-4.843314	3.134979	0.827730	C	0.448803	2.898521	-0.072849
H	-3.411120	5.255709	0.873198	C	1.316299	1.810822	0.153239
C	-5.942987	-0.702671	0.551269	C	0.972850	4.050363	-0.693696

C	2.653853	1.866367	-0.243591	C	3.157397	3.013311	-0.867764
H	0.945313	0.922629	0.669741	H	3.310252	1.013734	-0.052364
C	2.311494	4.105212	-1.089482	H	2.694246	5.005088	-1.577355
H	0.322999	4.906009	-0.891859	H	4.205528	3.058200	-1.173433



Zero-point correction=	0.329801 (Hartree/Particle)
Thermal correction to Energy=	0.348166
Thermal correction to Enthalpy=	0.349110
Thermal correction to Gibbs Free Energy=	0.283215
Sum of electronic and zero-point Energies=	-825.819866
Sum of electronic and thermal Energies=	-825.801501
Sum of electronic and thermal Enthalpies=	-825.800557
Sum of electronic and thermal Free Energies=	-825.866453

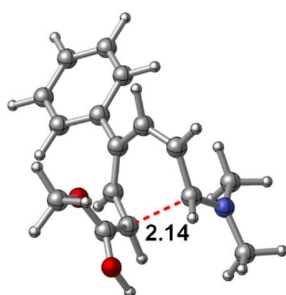
TS-3a-OH-du'

E(scf) = -826.147067192 a.u.

$\nu_{\min} = -231.47 \text{ cm}^{-1}$

C	-2.636233	2.672434	-1.571319	O	-5.131036	-0.429183	0.598073
C	-1.803647	2.527064	-0.362140	O	-3.310978	-0.252713	-0.652851
C	-2.327505	2.029299	0.786192	C	-4.848419	2.734444	-0.368193
H	-2.117115	2.732684	-2.531390	H	-5.688157	2.036503	-0.445310
H	-1.728972	2.057330	1.702414	H	-4.515823	2.935267	-2.512116
C	-3.687408	1.466057	0.906532	C	-3.739929	-1.440074	-1.353192
H	-4.205857	1.651023	1.853337	H	-3.815105	-2.285907	-0.656320
C	-3.974967	2.789612	-1.570782	H	-4.710772	-1.264199	-1.836334
C	-4.025236	0.238552	0.319771	H	-2.965417	-1.627217	-2.104081

N	-5.143362	3.842061	0.324944	C	0.623093	2.367700	0.302412
C	-6.228460	3.814873	1.298989	C	-0.055173	4.121682	-1.217788
H	-5.831379	3.643808	2.315450	C	1.936357	2.840738	0.261219
H	-6.755677	4.779822	1.292565	H	0.389424	1.476639	0.889436
H	-6.940542	3.016437	1.053511	C	1.258829	4.594710	-1.258259
C	-4.203460	4.946715	0.479001	H	-0.826878	4.641726	-1.790663
H	-4.760064	5.893940	0.518510	C	2.260125	3.957266	-0.518024
H	-3.633991	4.832038	1.417882	H	2.714267	2.326709	0.831438
H	-3.501733	4.974765	-0.361274	H	1.500411	5.468049	-1.869273
C	-0.398627	3.005178	-0.429268	H	3.288879	4.323998	-0.553715



Zero-point correction=	0.329273 (Hartree/Particle)
Thermal correction to Energy=	0.347898
Thermal correction to Enthalpy=	0.348842
Thermal correction to Gibbs Free Energy=	0.282046
Sum of electronic and zero-point Energies=	-825.817794
Sum of electronic and thermal Energies=	-825.799169
Sum of electronic and thermal Enthalpies=	-825.798225
Sum of electronic and thermal Free Energies=	-825.865022

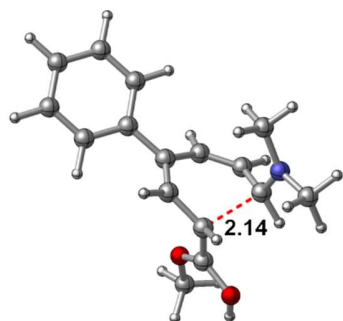
TS-3a-OH-ud'

E(scf) = -826.142578945 a.u.

$\nu_{\min} = -228.28 \text{ cm}^{-1}$

C	-1.666837	4.290178	0.619375	C	-2.948304	4.680521	0.507320
C	-1.128279	3.011390	0.116103	C	-3.737781	1.851723	1.686997
C	-1.940161	1.938831	-0.062327	O	-5.002732	1.597448	1.974162
H	-0.957633	4.985501	1.076063	O	-2.880929	2.175383	2.625068
H	-1.545444	1.046594	-0.559039	C	-4.047657	3.871750	-0.084582
C	-3.358814	1.895461	0.341996	H	-4.942815	3.778049	0.538341
H	-4.050604	1.351269	-0.306890	H	-3.257949	5.666245	0.871182

C	-3.278670	2.364071	3.994336	H	-6.310818	3.307896	-1.089389
H	-4.017365	3.176395	4.075583	C	0.312142	2.962428	-0.244392
H	-3.668264	1.427113	4.422856	C	1.064176	1.782268	-0.078401
H	-2.365990	2.647984	4.528736	C	0.960716	4.094985	-0.776365
N	-4.320319	3.929630	-1.394629	C	2.409888	1.731473	-0.447876
C	-3.292338	4.145459	-2.406361	H	0.594605	0.903031	0.368341
H	-2.939545	3.176776	-2.801228	C	2.307218	4.043638	-1.145804
H	-3.716437	4.729597	-3.235721	H	0.402533	5.022732	-0.924260
H	-2.441160	4.687575	-1.981029	C	3.037497	2.861492	-0.984427
C	-5.566789	3.360672	-1.894464	H	2.975366	0.807268	-0.304235
H	-5.959716	3.987496	-2.708150	H	2.787021	4.931655	-1.564903
H	-5.394702	2.344404	-2.291484	H	4.091948	2.822690	-1.268572



Zero-point correction=	0.328540 (Hartree/Particle)
Thermal correction to Energy=	0.347434
Thermal correction to Enthalpy=	0.348379
Thermal correction to Gibbs Free Energy=	0.280772
Sum of electronic and zero-point Energies=	-825.814039
Sum of electronic and thermal Energies=	-825.795145
Sum of electronic and thermal Enthalpies=	-825.794200
Sum of electronic and thermal Free Energies=	-825.861807

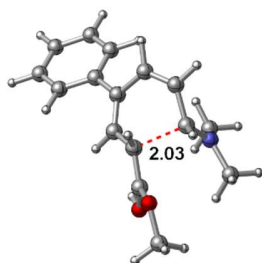
TS-3a-OH-uu'

E(scf) = -826.149706076 a.u.

$\nu_{\min} = -307.35 \text{ cm}^{-1}$

C	-1.410479	4.391634	0.930068	C	-2.593691	4.605233	0.323901
C	-1.131636	3.269447	1.840314	C	-3.922527	1.022625	0.829705
C	-1.896159	2.147435	1.769402	O	-4.379963	0.577554	1.978186
H	-1.759256	1.360121	2.519653	O	-4.568301	0.626326	-0.228130
C	-2.873745	1.954270	0.688554	C	-3.807749	3.740262	0.435456
H	-2.482058	1.992298	-0.334129	H	-4.233226	3.441481	-0.527685

H	-2.750047	5.513512	-0.268308	H	-6.286268	3.224056	0.168204
C	-5.733195	-0.222165	-0.101876	H	-0.620041	5.132773	0.787070
H	-5.464166	-1.159402	0.402954	C	-0.052128	3.423053	2.846335
H	-6.516898	0.299789	0.465379	C	0.716579	2.317714	3.263118
H	-6.062293	-0.413579	-1.128000	C	0.220578	4.679886	3.423142
N	-4.752900	4.067847	1.341893	C	1.710193	2.461113	4.233664
C	-4.435762	4.619765	2.653592	H	0.552248	1.341322	2.801637
H	-4.479057	3.832294	3.426267	C	1.215055	4.822256	4.393863
H	-3.433614	5.061558	2.653596	H	-0.365658	5.553442	3.128074
H	-5.169617	5.397876	2.912693	C	1.963268	3.713694	4.804225
C	-6.100542	3.527729	1.206745	H	2.299352	1.591921	4.536638
H	-6.245364	2.656703	1.869383	H	1.403538	5.804419	4.834460
H	-6.839080	4.293838	1.487106	H	2.744473	3.826346	5.559910



Zero-point correction=	0.329782 (Hartree/Particle)
Thermal correction to Energy=	0.348140
Thermal correction to Enthalpy=	0.349084
Thermal correction to Gibbs Free Energy=	0.283185
Sum of electronic and zero-point Energies=	-825.819924
Sum of electronic and thermal Energies=	-825.801566
Sum of electronic and thermal Enthalpies=	-825.800622
Sum of electronic and thermal Free Energies=	-825.866521

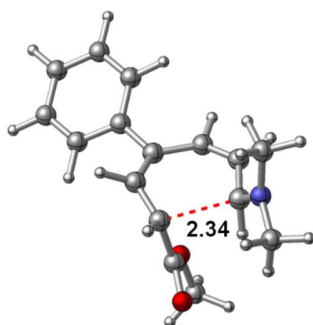
TS-3a-ud

E(scf) = -825.713904076 a.u.

$\nu_{\min} = -318.43 \text{ cm}^{-1}$

C	-1.426196	4.395015	0.002069	H	-1.163486	1.152685	-0.884617
C	-0.849189	3.078609	-0.045118	C	-3.022700	1.833525	-0.032254
C	-1.636196	1.966301	-0.316833	H	-3.589038	1.131648	-0.654120
H	-0.706888	5.217415	0.060694	C	-2.715314	4.780640	-0.266952

C	-3.568043	1.840546	1.325680	C	-6.194646	3.545291	-0.987137
O	-4.646174	1.354093	1.637436	H	-6.976911	4.268877	-1.269099
O	-2.792119	2.480689	2.232462	H	-6.331609	2.635394	-1.599691
C	-3.919992	3.977615	-0.258089	H	-6.319655	3.269573	0.068007
H	-4.323273	3.721235	0.717479	C	0.630771	2.937575	-0.083206
H	-2.861194	5.818993	-0.590361	C	1.231711	1.769870	0.433551
C	-3.288433	2.536803	3.567820	C	1.482367	3.918552	-0.635429
H	-4.260647	3.052784	3.609050	C	2.616360	1.584815	0.392700
H	-3.414647	1.526680	3.988016	H	0.598375	1.009050	0.896107
H	-2.542933	3.094380	4.148889	C	2.866940	3.738950	-0.668380
N	-4.873689	4.112328	-1.201866	H	1.057111	4.824940	-1.071776
C	-4.567186	4.491921	-2.570349	C	3.443213	2.570274	-0.156141
H	-4.806866	3.661704	-3.259204	H	3.052134	0.670601	0.804730
H	-5.159114	5.370856	-2.875387	H	3.500554	4.513358	-1.109185
H	-3.501658	4.733490	-2.669428	H	4.526963	2.431230	-0.183096



Zero-point correction=	0.315350 (Hartree/Particle)
Thermal correction to Energy=	0.334113
Thermal correction to Enthalpy=	0.335057
Thermal correction to Gibbs Free Energy=	0.266729
Sum of electronic and zero-point Energies=	-825.398554
Sum of electronic and thermal Energies=	-825.379791
Sum of electronic and thermal Enthalpies=	-825.378847
Sum of electronic and thermal Free Energies=	-825.447175

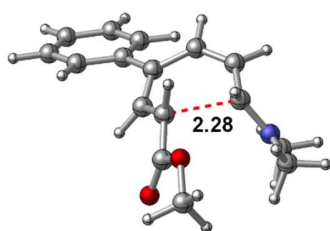
TS-3a-uu

E(scf) = -825.722678629 a.u.

$\nu_{\min} = -268.29 \text{ cm}^{-1}$

C	-1.475648	4.685812	1.460235	H	-1.950017	1.787563	3.052562
C	-1.053997	3.468102	2.053679	C	-2.904344	2.102290	1.159788
C	-1.938927	2.379327	2.131220	H	-2.596550	2.112460	0.118067

C	-2.771869	4.994599	1.045469	C	-6.089182	3.775512	-0.166988
C	-4.005231	1.156088	1.489633	H	-5.937323	2.697448	-0.044846
O	-4.362270	0.878574	2.615246	H	-7.122749	4.050413	0.071615
O	-4.597113	0.680350	0.382787	H	-5.844677	4.073126	-1.193362
C	-3.733904	4.105369	0.541553	H	-0.815413	5.543925	1.609022
H	-3.623007	3.629552	-0.425361	C	0.196760	3.431712	2.857317
H	-3.093857	6.025537	1.254038	C	0.902232	2.216218	2.966964
C	-5.681033	-0.242253	0.578587	C	0.708234	4.562024	3.526205
H	-5.331785	-1.132904	1.120843	C	2.079858	2.133738	3.713201
H	-6.490983	0.230533	1.154140	H	0.532713	1.333035	2.440489
H	-6.030843	-0.516069	-0.423161	C	1.886047	4.479078	4.270845
N	-5.165238	4.489258	0.773012	H	0.168905	5.510731	3.492668
C	-5.559350	4.290918	2.211412	C	2.577408	3.265790	4.366534
H	-5.484443	3.223938	2.450983	H	2.614689	1.183053	3.777662
H	-4.868503	4.859647	2.843873	H	2.260593	5.365260	4.788973
H	-6.586115	4.650326	2.347477	H	3.499404	3.203679	4.949693



Zero-point correction=	0.315729 (Hartree/Particle)
Thermal correction to Energy=	0.334345
Thermal correction to Enthalpy=	0.335289
Thermal correction to Gibbs Free Energy=	0.267895
Sum of electronic and zero-point Energies=	-825.406950
Sum of electronic and thermal Energies=	-825.388333
Sum of electronic and thermal Enthalpies=	-825.387389
Sum of electronic and thermal Free Energies=	-825.454784

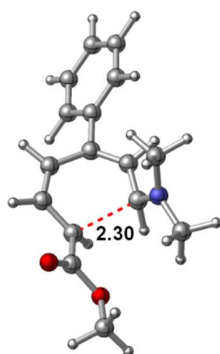
TS-3b-dd

E(scf) = -825.719040934 a.u.

$\nu_{\min} = -276.49 \text{ cm}^{-1}$

C	-1.547054	4.106997	0.269649	C	-2.850816	1.548967	0.581097
C	-0.823768	2.863735	0.199963	H	-3.075396	1.991090	1.550823
C	-1.527881	1.668159	0.107577	C	-2.880299	4.344852	0.022586
H	-0.931139	5.009511	0.331151	C	-3.693194	0.431215	0.170332
H	-1.080183	0.814194	-0.414938	O	-3.460844	-0.360195	-0.728004

O	-4.852664	0.392207	0.883719	C	-6.099912	2.798925	-1.142756
C	-3.988156	3.407018	-0.079620	H	-6.852846	3.511498	-1.519268
H	-4.508882	3.093769	0.821668	H	-6.134182	1.897497	-1.779443
H	-3.135298	5.365426	-0.292144	H	-6.360119	2.511018	-0.116774
C	-5.792044	-0.612710	0.510099	C	0.646584	2.880512	-0.001007
H	-6.127548	-0.472052	-0.530238	C	1.431007	1.788002	0.430165
H	-5.354365	-1.619034	0.598963	C	1.317247	3.949686	-0.635024
H	-6.644026	-0.510704	1.194103	C	2.813113	1.759016	0.228637
N	-4.773633	3.394766	-1.173988	H	0.946812	0.959418	0.952481
C	-4.291287	3.794043	-2.486307	C	2.700809	3.927304	-0.825118
H	-4.465525	2.982333	-3.213256	H	0.746895	4.801668	-1.011317
H	-4.817342	4.694787	-2.845951	C	3.458695	2.831002	-0.397132
H	-3.215981	4.008468	-2.442312	H	3.391518	0.898786	0.576597



Zero-point correction=	0.315421 (Hartree/Particle)
Thermal correction to Energy=	0.334124
Thermal correction to Enthalpy=	0.335069
Thermal correction to Gibbs Free Energy=	0.267411
Sum of electronic and zero-point Energies=	-825.403620
Sum of electronic and thermal Energies=	-825.384916
Sum of electronic and thermal Enthalpies=	-825.383972
Sum of electronic and thermal Free Energies=	-825.451630

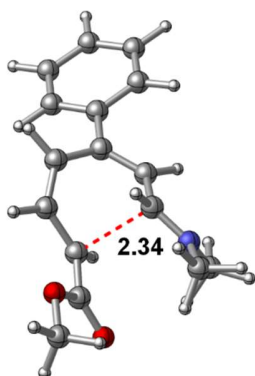
TS-3b-du

E(scf) = -825.711208173 a.u.

$\nu_{\min} = -604.51 \text{ cm}^{-1}$

C	-1.825050	4.186135	0.848739	H	-1.664171	0.982769	-0.401062
C	-1.251318	2.961139	0.268977	C	-3.336650	1.678047	0.778941
C	-2.038841	1.825142	0.191413	H	-3.558946	2.170960	1.726443
H	-1.152864	4.869300	1.379900	C	-3.132471	4.527591	0.765824

C	-4.316408	0.720803	0.379879	H	-5.371885	4.609845	2.036886
O	-5.422861	0.559859	0.905017	C	-6.253746	3.140284	-0.901967
O	-3.966396	0.010665	-0.743264	H	-6.667735	2.201740	-0.507673
C	-4.071772	3.738376	-0.053605	H	-7.073152	3.834686	-1.142405
H	-3.722556	3.443866	-1.049290	H	-5.679950	2.925772	-1.811718
H	-3.508344	5.431781	1.249486	C	0.135574	2.995644	-0.228194
C	-4.936512	-0.897438	-1.243924	C	0.921841	1.823424	-0.336370
H	-5.234683	-1.635257	-0.481839	C	0.739064	4.212486	-0.626010
H	-5.845186	-0.370380	-1.580875	C	2.223736	1.863951	-0.837280
H	-4.472627	-1.410673	-2.097135	H	0.513007	0.868716	0.001940
N	-5.381921	3.748677	0.104032	C	2.047554	4.253367	-1.112933
C	-6.006217	3.980550	1.402850	H	0.164383	5.140826	-0.577723
H	-6.981305	4.466787	1.261530	C	2.800415	3.079282	-1.227619
H	-6.150648	3.003214	1.893068	H	2.801817	0.938065	-0.906024



Zero-point correction=	0.315298 (Hartree/Particle)
Thermal correction to Energy=	0.333914
Thermal correction to Enthalpy=	0.334858
Thermal correction to Gibbs Free Energy=	0.267777
Sum of electronic and zero-point Energies=	-825.395910
Sum of electronic and thermal Energies=	-825.377295
Sum of electronic and thermal Enthalpies=	-825.376350
Sum of electronic and thermal Free Energies=	-825.443432

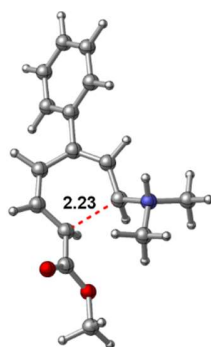
TS-3b-H-dd

E(scf) = -826.137686527 a.u.

ν_{\min} = -452.60cm⁻¹

C	-1.542681	4.262377	0.310911	C	-0.874921	3.007683	0.383310
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C	-1.471530	1.787860	0.113027	C	-5.287790	2.310449	-1.982795
H	-0.881364	1.000890	-0.368424	H	-5.798090	1.764595	-1.181939
C	-2.839293	1.562487	0.335683	H	-5.975491	2.503304	-2.814502
H	-3.239160	1.882026	1.294466	H	-4.416895	1.744427	-2.330597
C	-2.830358	4.385578	-0.236228	C	-5.973409	4.517357	-1.069011
C	-3.476508	0.343916	-0.229660	H	-6.589103	4.682431	-1.961783
O	-3.018428	-0.325067	-1.131150	H	-6.562052	4.020487	-0.288353
O	-4.656627	0.093712	0.360511	H	-5.578430	5.469355	-0.696420
C	-3.870753	3.440168	-0.279673	H	0.217350	3.056880	0.390095
H	-4.451894	3.157078	0.591954	C	-0.715786	5.489015	0.515662
H	-3.000280	5.304159	-0.812521	C	-0.789216	6.610163	-0.332783
C	-5.375732	-1.058231	-0.103828	C	0.176443	5.531679	1.603947
H	-5.615752	-0.959312	-1.173493	C	0.003770	7.735095	-0.098913
H	-4.777087	-1.969264	0.041661	H	-1.448506	6.602555	-1.203517
H	-6.294519	-1.104259	0.491746	C	0.963369	6.661340	1.842484
N	-4.818921	3.624636	-1.432352	H	0.239785	4.677531	2.282552



Zero-point correction=	0.331508 (Hartree/Particle)
Thermal correction to Energy=	0.349798
Thermal correction to Enthalpy=	0.350742
Thermal correction to Gibbs Free Energy=	0.283867
Sum of electronic and zero-point Energies=	-825.806179
Sum of electronic and thermal Energies=	-825.787888
Sum of electronic and thermal Enthalpies=	-825.786944
Sum of electronic and thermal Free Energies=	-825.853820

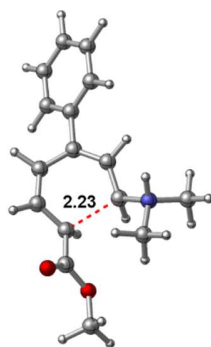
TS-3b-H-du

E(scf) = -826.134270537 a.u.

$\nu_{\min} = -450.87 \text{ cm}^{-1}$

C	-2.136646	4.175484	0.329866	H	-1.672606	1.882950	2.730891
C	-1.532104	3.077089	0.993351	C	-3.518147	1.700045	1.661624
C	-2.197709	2.171720	1.810779	H	-4.019818	1.369542	2.577599

C	-3.521395	4.416248	0.422986	H	-7.593665	3.130657	1.937942
C	-3.937402	0.825403	0.532638	H	-6.544435	1.864136	1.191369
O	-4.915059	0.106085	0.584506	C	-6.687233	4.303585	-0.219850
O	-3.151156	0.921455	-0.546534	H	-6.850729	3.434273	-0.868175
C	-4.500761	3.427356	0.522556	H	-7.645238	4.690306	0.148171
H	-4.592492	2.695516	-0.273477	H	-6.140674	5.084014	-0.761072
H	-3.822111	5.466200	0.533646	H	-0.446832	3.135613	1.110763
C	-3.502421	0.110324	-1.677541	C	-1.286803	5.272067	-0.207883
H	-3.465299	-0.956235	-1.412060	C	-1.746929	6.010543	-1.317022
H	-4.515110	0.355731	-2.030556	C	-0.036472	5.611437	0.347166
H	-2.761485	0.337240	-2.452550	C	-0.982614	7.047527	-1.857049
N	-5.857924	3.861422	0.956494	H	-2.703074	5.748540	-1.776456
C	-6.563499	2.802454	1.757843	C	0.726007	6.648314	-0.192680
H	-6.032550	2.675073	2.706729	H	0.335193	5.083492	1.227455



Zero-point correction=	0.331511 (Hartree/Particle)
Thermal correction to Energy=	0.349630
Thermal correction to Enthalpy=	0.350574
Thermal correction to Gibbs Free Energy=	0.284589
Sum of electronic and zero-point Energies=	-825.802759
Sum of electronic and thermal Energies=	-825.784640
Sum of electronic and thermal Enthalpies=	-825.783696
Sum of electronic and thermal Free Energies=	-825.849681

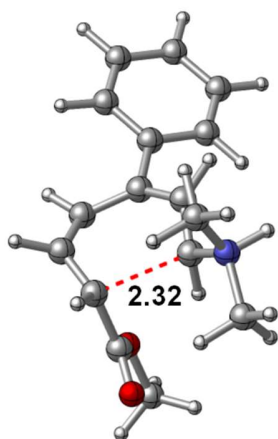
TS-3b-H-ud

E(scf) = -826.134117172 a.u.

$\nu_{\min} = -462.23 \text{ cm}^{-1}$

C	-1.362173	4.544251	0.214540	C	-3.042853	1.925962	-0.281644
C	-0.918540	3.201603	0.131098	H	-3.502552	1.318830	-1.070064
C	-1.656180	2.138666	-0.385703	C	-2.658972	4.912112	-0.203955
H	-1.102247	1.453162	-1.041107	C	-3.729876	1.651844	1.009200

O	-4.803121	1.086472	1.074443	H	-3.850665	4.761668	-2.657240
O	-3.063256	2.091858	2.083862	C	-6.206082	3.711110	-0.405271
C	-3.788419	4.113753	-0.060185	H	-7.050610	3.974928	-1.051512
H	-4.074066	3.783556	0.931384	H	-6.003930	2.634606	-0.444611
H	-2.735691	5.843527	-0.778818	H	-6.411412	4.011710	0.628975
C	-3.668568	1.853699	3.363662	H	0.164136	3.059533	0.186411
H	-4.658543	2.330486	3.418901	C	-0.378867	5.639028	0.433321
H	-3.781243	0.774125	3.540360	C	-0.807141	6.821817	1.069683
H	-2.990355	2.293327	4.103854	C	0.967388	5.551123	0.025355
N	-4.987393	4.443347	-0.886211	C	0.078984	7.877482	1.296322
C	-4.747524	4.212229	-2.351001	H	-1.841219	6.901648	1.413522
H	-4.599552	3.137474	-2.503753	C	1.851801	6.606846	0.251618
H	-5.621085	4.567481	-2.910081	H	1.325183	4.664495	-0.501494



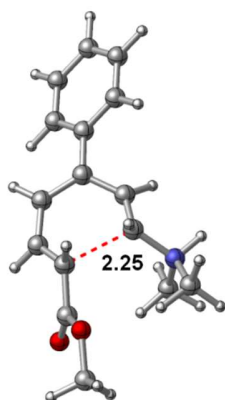
Zero-point correction=	0.331202 (Hartree/Particle)
Thermal correction to Energy=	0.349383
Thermal correction to Enthalpy=	0.350328
Thermal correction to Gibbs Free Energy=	0.284409
Sum of electronic and zero-point Energies=	-825.802915
Sum of electronic and thermal Energies=	-825.784734
Sum of electronic and thermal Enthalpies=	-825.783790
Sum of electronic and thermal Free Energies=	-825.849708

TS-3b-H-uu

E(scf) = -826.140727266 a.u.

$\nu_{\min} = -464.38 \text{ cm}^{-1}$

C	-1.353401	4.564919	1.216503	N	-5.090750	4.493171	0.670013
C	-1.040355	3.291752	1.756961	C	-5.446280	4.372862	2.126156
C	-1.943536	2.248399	1.914730	H	-5.404860	3.315544	2.410808
H	-1.861837	1.631196	2.817001	H	-4.716652	4.940939	2.713834
C	-3.019076	2.001600	1.045274	H	-6.454168	4.777667	2.275141
H	-2.807227	1.940590	-0.017788	C	-6.068609	3.773385	-0.209413
C	-2.679872	4.911489	0.882976	H	-5.959078	2.696960	-0.038446
C	-4.124844	1.124751	1.515251	H	-7.082025	4.105109	0.043294
O	-4.387671	0.910368	2.680380	H	-5.842069	4.012023	-1.255348
O	-4.839454	0.632379	0.489586	H	-0.101473	3.226835	2.312665
C	-3.679381	4.059572	0.403441	C	-0.366005	5.675056	1.307745
H	-3.607284	3.587530	-0.569198	C	0.600903	5.755842	2.329982
H	-2.977803	5.928005	1.174238	C	-0.397057	6.696380	0.336858
C	-5.940719	-0.226048	0.826572	C	1.504145	6.818819	2.374937
H	-5.581998	-1.112436	1.369755	H	0.633795	5.000613	3.117411
H	-6.667946	0.307721	1.456582	C	0.508377	7.759190	0.381918
H	-6.398985	-0.519466	-0.124658	H	-1.123698	6.640388	-0.477268



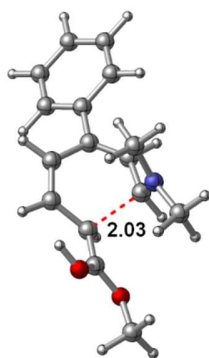
Zero-point correction=	0.331649 (Hartree/Particle)
Thermal correction to Energy=	0.349785
Thermal correction to Enthalpy=	0.350730
Thermal correction to Gibbs Free Energy=	0.284833
Sum of electronic and zero-point Energies=	-825.809078
Sum of electronic and thermal Energies=	-825.790942
Sum of electronic and thermal Enthalpies=	-825.789998
Sum of electronic and thermal Free Energies=	-825.855894

TS-3b-OH-dd'

E(scf) = -826.148431900 a.u.

$v_{\min} = -318.87 \text{ cm}^{-1}$

C	-1.699789	4.302640	0.139861	H	-4.520623	4.188121	-3.188866
C	-1.091762	3.030920	-0.283235	H	-2.988131	4.216815	-2.269526
C	-1.721128	1.843961	-0.172074	C	-5.885780	2.629528	-1.472174
H	-1.241709	0.945121	-0.577580	H	-5.718495	1.619665	-1.885053
C	-3.013648	1.734280	0.527101	H	-6.424133	2.543579	-0.519245
H	-3.024769	2.060323	1.572894	H	-6.514664	3.186728	-2.182902
C	-3.046778	4.425905	0.244539	H	-0.098786	3.074541	-0.736382
C	-3.872497	0.644535	0.289048	C	-0.798194	5.460155	0.388088
O	-3.844009	-0.112661	-0.785347	C	-1.176965	6.773992	0.051749
O	-4.838894	0.399626	1.126169	C	0.465428	5.256840	0.975006
C	-4.067117	3.375099	-0.046140	C	-0.325678	7.850547	0.308575
H	-4.806163	3.242002	0.750120	H	-2.136719	6.952937	-0.438230
H	-3.491307	5.387725	0.519597	C	1.315084	6.334898	1.235914
C	-5.811016	-0.632992	0.841989	H	0.779911	4.246853	1.248919
H	-6.361025	-0.387536	-0.077556	C	0.922582	7.635737	0.904164
H	-5.309307	-1.603526	0.732178	H	-0.634326	8.861917	0.032691
H	-6.484936	-0.639175	1.704376	H	2.287533	6.157135	1.701657
N	-4.622396	3.330175	-1.276274	H	1.589170	8.478597	1.102487
C	-3.879693	3.622203	-2.495912	H	-3.095270	0.099882	-1.368546
H	-3.569880	2.688138	-2.996599				



Zero-point correction=	0.329477 (Hartree/Particle)
Thermal correction to Energy=	0.347983
Thermal correction to Enthalpy=	0.348927
Thermal correction to Gibbs Free Energy=	0.282336
Sum of electronic and zero-point Energies=	-825.818955
Sum of electronic and thermal Energies=	-825.800449
Sum of electronic and thermal Enthalpies=	-825.799505

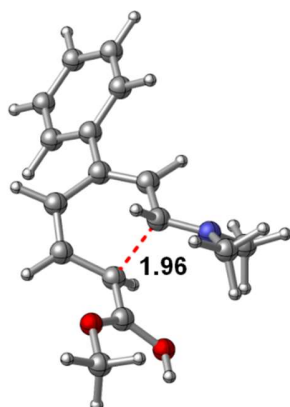
Sum of electronic and thermal Free Energies= -825.866096

TS-3b-OH-du'

E(scf) = -826.143737584 a.u.

$\nu_{\min} = -393.10\text{cm}^{-1}$

C	-2.067592	4.467961	-0.313668	N	-5.567331	3.297520	-0.109783
C	-1.341620	3.192514	-0.166296	C	-6.475816	2.284428	-0.628968
C	-1.888905	2.117522	0.431114	H	-5.958601	1.649293	-1.360385
H	-1.326542	1.182295	0.498635	H	-6.876294	1.648460	0.177150
C	-3.253867	2.166905	1.021257	H	-7.328478	2.770576	-1.130549
H	-3.398942	2.858959	1.859512	C	-6.108125	4.132030	0.953197
C	-3.424073	4.456501	-0.311295	H	-5.441424	4.975622	1.169199
C	-3.969697	0.968647	1.185302	H	-7.090283	4.526326	0.652453
O	-5.018703	0.968295	1.980038	H	-6.235800	3.546637	1.881599
O	-3.639915	-0.078650	0.475169	H	-0.318352	3.135365	-0.544292
C	-4.229355	3.201152	-0.328361	C	-1.290976	5.725211	-0.446003
H	-3.983520	2.534701	-1.167354	C	-1.779042	6.813360	-1.196947
H	-3.985359	5.390706	-0.366365	C	-0.040935	5.859585	0.190027
C	-4.381895	-1.313994	0.527767	C	-1.049505	7.999221	-1.294571
H	-4.349400	-1.738281	1.542943	H	-2.727150	6.721009	-1.731330
H	-5.418927	-1.160257	0.191487	C	0.686694	7.048350	0.094983
H	-3.872057	-1.990601	-0.165654	H	0.357944	5.034184	0.784204



Zero-point correction= 0.328909 (Hartree/Particle)

Thermal correction to Energy= 0.347614

Thermal correction to Enthalpy= 0.348558

Thermal correction to Gibbs Free Energy= 0.281824

Sum of electronic and zero-point Energies= -825.814828

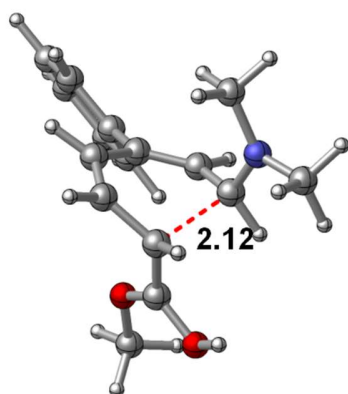
Sum of electronic and thermal Energies= -825.796123
 Sum of electronic and thermal Enthalpies= -825.795179
 Sum of electronic and thermal Free Energies= -825.861913

TS-3b-OH-ud'

E(scf) = -826.146344756 a.u.

$\nu_{\min} = -239.51\text{cm}^{-1}$

C	-1.797971	4.521436	0.022530	N	-4.820461	3.951592	-1.357924
C	-1.372698	3.250986	-0.592003	C	-4.055883	4.193955	-2.574873
C	-2.112009	2.127090	-0.575851	H	-3.739306	3.236982	-3.025640
H	-1.753267	1.239488	-1.107680	H	-4.686633	4.731014	-3.297965
C	-3.404385	2.010119	0.137570	H	-3.166660	4.794903	-2.354729
H	-4.171392	1.392169	-0.340635	C	-6.115703	3.313970	-1.558424
C	-3.108674	4.815566	0.190253	H	-6.707467	3.895611	-2.280286
C	-3.453306	1.979940	1.539135	H	-5.989202	2.292123	-1.959256
O	-4.522646	1.631087	2.230918	H	-6.663767	3.258761	-0.608760
O	-2.463114	2.445555	2.245747	H	-0.397235	3.231109	-1.083181
C	-4.254944	3.929976	-0.139643	C	-0.750539	5.486921	0.451120
H	-4.989968	3.825987	0.665729	C	-0.867169	6.155659	1.684785
H	-3.404710	5.787620	0.598382	C	0.374563	5.751768	-0.352800
C	-2.576699	2.577257	3.678915	C	0.103314	7.072546	2.095421
H	-3.408858	3.248250	3.931674	H	-1.715532	5.934264	2.336501
H	-2.734454	1.592353	4.139118	C	1.340828	6.674203	0.055995
H	-1.623909	3.007993	4.003528	H	0.487030	5.254776	-1.318910



Zero-point correction= 0.329256 (Hartree/Particle)
 Thermal correction to Energy= 0.347878

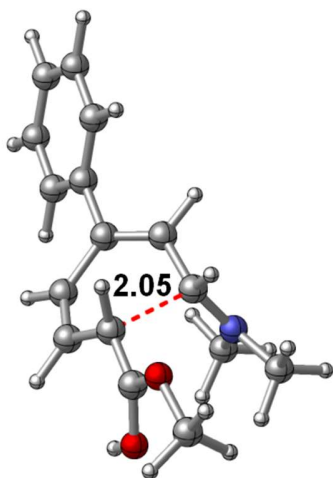
Thermal correction to Enthalpy=	0.348822
Thermal correction to Gibbs Free Energy=	0.282088
Sum of electronic and zero-point Energies=	-825.817089
Sum of electronic and thermal Energies=	-825.798467
Sum of electronic and thermal Enthalpies=	-825.797523
Sum of electronic and thermal Free Energies=	-825.864256

TS-3b-OH-uu'

E(scf) = -826.147456903 a.u.

$\nu_{\min} = -288.49\text{cm}^{-1}$

C	-1.616855	4.639521	1.350444	N	-4.978779	4.135521	1.261724
C	-1.478307	3.525118	2.298753	C	-4.892741	4.734812	2.587851
C	-2.142760	2.359656	2.161237	H	-5.012728	3.963974	3.369094
H	-2.034119	1.590149	2.934848	H	-3.925692	5.231381	2.722207
C	-2.942046	2.080760	0.956225	H	-5.696456	5.476805	2.708508
H	-2.405371	2.118008	0.002110	C	-6.263445	3.526007	0.939670
C	-2.719310	4.762877	0.568929	H	-6.472704	2.673198	1.608222
C	-3.960846	1.111230	0.969747	H	-7.069372	4.264283	1.068359
O	-4.568081	0.674207	2.051470	H	-6.268145	3.176868	-0.101020
O	-4.427038	0.658931	-0.159314	H	-0.802361	3.655434	3.145889
C	-3.893651	3.844743	0.516631	C	-0.550247	5.678464	1.304546
H	-4.153462	3.500759	-0.489580	C	0.060431	6.149212	2.482608
H	-2.853290	5.662355	-0.041762	C	-0.137218	6.220747	0.072627
C	-5.553848	-0.247228	-0.176663	C	1.039640	7.144352	2.429891
H	-5.314322	-1.158418	0.387474	H	-0.247139	5.757301	3.454517
H	-6.436806	0.242543	0.257905	C	0.846212	7.211295	0.020743
H	-5.721890	-0.477702	-1.233376	H	-0.576360	5.845001	-0.854405



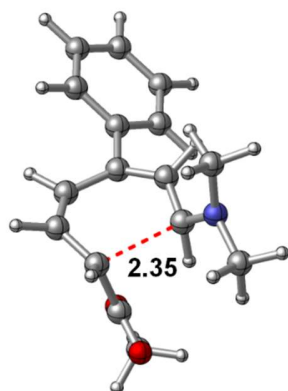
Zero-point correction=	0.329313 (Hartree/Particle)
Thermal correction to Energy=	0.347853
Thermal correction to Enthalpy=	0.348797
Thermal correction to Gibbs Free Energy=	0.282244
Sum of electronic and zero-point Energies=	-825.818144
Sum of electronic and thermal Energies=	-825.799604
Sum of electronic and thermal Enthalpies=	-825.798660
Sum of electronic and thermal Free Energies=	-825.865213

TS-3b-ud

E(scf) = -825.711936346 a.u.

$\nu_{\min} = -334.00\text{cm}^{-1}$

C	-1.425807	4.442958	0.218764	N	-4.907847	4.194016	-0.997581
C	-0.905098	3.107922	0.101912	C	-4.630176	4.595298	-2.366625
C	-1.628663	2.002677	-0.279339	H	-4.703113	3.724358	-3.045779
H	-1.082590	1.218903	-0.824736	H	-5.357664	5.352222	-2.700303
C	-3.032504	1.815431	-0.105978	H	-3.621434	5.016586	-2.450226
H	-3.533491	1.159932	-0.827620	C	-6.181264	3.520553	-0.802909
C	-2.727855	4.810935	-0.077850	H	-7.007442	4.159017	-1.153167
C	-3.662647	1.672518	1.204480	H	-6.213473	2.570488	-1.369154
O	-4.747699	1.141414	1.395391	H	-6.329537	3.285947	0.259115
O	-2.956645	2.224140	2.224145	H	0.185054	3.023783	0.090651
C	-3.916527	3.997083	-0.097974	C	-0.446218	5.554970	0.422498
H	-4.279644	3.662893	0.869207	C	-0.792796	6.647639	1.241459
H	-2.876843	5.844144	-0.413075	C	0.823681	5.564112	-0.187822
C	-3.541761	2.136852	3.521319	C	0.094382	7.708428	1.445069
H	-4.522467	2.637646	3.549760	H	-1.765861	6.650410	1.738259
H	-3.679934	1.087610	3.825959	C	1.710382	6.624840	0.012954
H	-2.845570	2.637642	4.206112	H	1.113904	4.745124	-0.849381



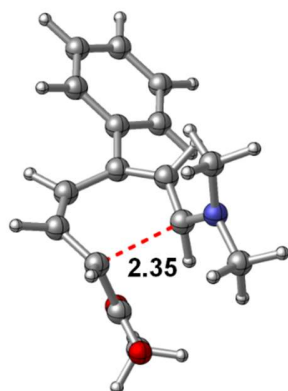
Zero-point correction=	0.315371 (Hartree/Particle)
Thermal correction to Energy=	0.334058
Thermal correction to Enthalpy=	0.335002
Thermal correction to Gibbs Free Energy=	0.267122
Sum of electronic and zero-point Energies=	-825.396565
Sum of electronic and thermal Energies=	-825.377879
Sum of electronic and thermal Enthalpies=	-825.376934
Sum of electronic and thermal Free Energies=	-825.444814

TS-3b-uu

E(scf) = -825.719525678 a.u.

$\nu_{\min} = -292.22\text{cm}^{-1}$

C	-1.422207	4.469523	1.262841	N	-5.042100	4.189452	1.022262
C	-1.050753	3.254791	1.934769	C	-5.212285	4.922239	2.265601
C	-1.856240	2.138812	1.988745	H	-5.858497	4.350218	2.953609
H	-1.771928	1.447589	2.836894	H	-4.237883	5.082347	2.744770
C	-2.838093	1.891962	1.000525	H	-5.684457	5.904458	2.090813
H	-2.533585	2.014737	-0.037058	C	-6.254479	3.631609	0.447019
C	-2.694107	4.757677	0.778512	H	-6.743678	2.944641	1.160183
C	-3.927736	0.954629	1.242733	H	-6.971824	4.432910	0.200716
O	-4.238969	0.465902	2.316173	H	-6.016730	3.071576	-0.465742
O	-4.641882	0.715042	0.107875	H	-0.162511	3.296482	2.569903
C	-3.824932	3.889596	0.518610	C	-0.456403	5.612467	1.302562
H	-3.879914	3.343473	-0.419172	C	0.325462	5.896350	2.439683
H	-2.952787	5.823688	0.751424	C	-0.319333	6.453417	0.180951
C	-5.791171	-0.115824	0.247735	C	1.207850	6.979433	2.453586
H	-5.519698	-1.108513	0.639110	H	0.225524	5.279466	3.335231
H	-6.524687	0.337449	0.934333	C	0.565620	7.535508	0.192317
H	-6.228258	-0.212651	-0.754161	H	-0.904805	6.240031	-0.716466



Zero-point correction=	0.315467 (Hartree/Particle)
Thermal correction to Energy=	0.334150
Thermal correction to Enthalpy=	0.335094
Thermal correction to Gibbs Free Energy=	0.267470
Sum of electronic and zero-point Energies=	-825.404059
Sum of electronic and thermal Energies=	-825.385376
Sum of electronic and thermal Enthalpies=	-825.384431
Sum of electronic and thermal Free Energies=	-825.452055

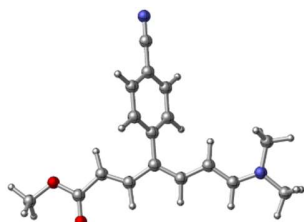
3a-CN

E(scf) = -917.942063716 a.u.

$\nu_{\min} = 30.77 \text{ cm}^{-1}$

C	-0.161761	2.243007	0.424137	H	-6.846675	-0.808015	-0.658667
C	-1.497747	2.604919	0.383825	H	-7.812986	0.528538	-1.382774
C	-2.461018	1.635273	-0.071618	N	3.352013	3.114793	1.243359
H	0.066752	1.225352	0.082948	C	3.301319	4.470753	1.766198
H	-2.060506	0.645789	-0.322820	H	2.868757	5.163729	1.024866
C	-3.802148	1.795434	-0.248720	H	2.686839	4.521756	2.681600
H	-4.310927	2.738940	-0.045631	H	4.316441	4.808717	2.008175
C	0.945400	3.011830	0.873973	C	4.646467	2.453855	1.191531
C	-4.624368	0.687955	-0.738605	H	5.351039	3.020123	0.559207
O	-4.241373	-0.437606	-1.012599	H	5.084642	2.365641	2.200417
O	-5.922641	1.057609	-0.865020	H	4.536728	1.445268	0.771750
C	2.225941	2.494731	0.847026	C	-1.947876	3.964108	0.796233
H	2.374586	1.478105	0.467539	C	-2.889063	4.130762	1.831222
H	0.770653	4.020119	1.252125	C	-1.445002	5.116723	0.161978
C	-6.822561	0.058148	-1.338866	C	-3.310131	5.397320	2.226970
H	-6.529146	-0.297101	-2.339437	H	-3.290026	3.249693	2.336012

C	-1.856180	6.390641	0.545710	H	-4.034792	5.508516	3.035851
H	-0.723001	5.006805	-0.649634	H	-1.458840	7.272941	0.040219
C	-2.794444	6.540349	1.585105	C	-3.223029	7.849033	1.987253



Zero-point correction= 0.315475 (Hartree/Particle)

Thermal correction to Energy= 0.336941

Thermal correction to Enthalpy= 0.337885

Thermal correction to Gibbs Free Energy= 0.262229

Sum of electronic and zero-point Energies= -917.626589

Sum of electronic and thermal Energies= -917.605123

Sum of electronic and thermal Enthalpies= -917.604179

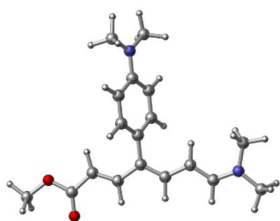
Sum of electronic and thermal Free Energies= -917.6798

3a-NMe₂

E(scf) = -959.644321276 a.u.

$\nu_{\min} = 22.16 \text{ cm}^{-1}$

C	-0.158732	2.216616	0.411813	C	3.289891	4.469058	1.761959
C	-1.491391	2.586337	0.377554	H	2.815251	5.155933	1.040924
C	-2.450783	1.615659	-0.083908	H	2.704351	4.501788	2.698020
H	0.073385	1.203802	0.057546	H	4.303769	4.832186	1.971933
H	-2.052807	0.625593	-0.338278	C	4.650113	2.457413	1.211995
C	-3.793529	1.778813	-0.254769	H	5.382274	3.037032	0.624644
H	-4.293786	2.724149	-0.039976	H	5.049550	2.337816	2.234621
C	0.948946	2.988883	0.865667	H	4.555911	1.460948	0.760167
C	-4.622103	0.679048	-0.745427	C	-1.941073	3.947700	0.790564
O	-4.248608	-0.448254	-1.028614	C	-2.864438	4.135538	1.834499
O	-5.921769	1.054322	-0.862850	C	-1.463447	5.107298	0.155408
C	2.232465	2.487316	0.832241	C	-3.287096	5.402390	2.232263
H	2.392912	1.474513	0.446944	H	-3.263462	3.261676	2.356353
H	0.760831	3.992671	1.249714	C	-1.871677	6.384726	0.535733
C	-6.826517	0.060303	-1.336393	H	-0.750603	5.006863	-0.667519
H	-6.540565	-0.291461	-2.340522	C	-2.799562	6.573137	1.593498
H	-6.849943	-0.809862	-0.661051	H	-4.001348	5.476148	3.051530
H	-7.816243	0.533191	-1.372526	H	-1.465341	7.239988	-0.003075
N	3.357169	3.120376	1.226766	N	-3.209272	7.832704	1.981396



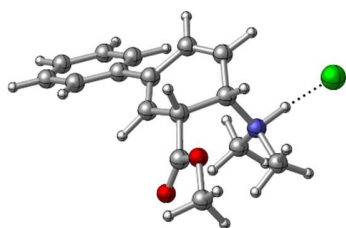
Zero-point correction=	0.388933 (Hartree/Particle)
Thermal correction to Energy=	0.413152
Thermal correction to Enthalpy=	0.414096
Thermal correction to Gibbs Free Energy=	0.331359
Sum of electronic and zero-point Energies=	-959.255389
Sum of electronic and thermal Energies=	-959.231170
Sum of electronic and thermal Enthalpies=	-959.230225
Sum of electronic and thermal Free Energies=	-959.312963

3a-OH-Cl

E(scf) = -1286.46489884 a.u.

$\nu_{\min} = 21.77 \text{ cm}^{-1}$

C	-1.372853	4.504752	0.954385	H	-4.333828	3.257382	3.105109
C	-1.134815	3.384607	1.885571	H	-3.455857	4.787617	2.755838
C	-1.957787	2.313829	1.818970	H	-5.205979	4.832072	3.111116
H	-1.878377	1.483026	2.521678	C	-6.051326	3.491792	0.985713
C	-2.996139	2.214186	0.735142	H	-6.154639	2.575687	1.579330
H	-2.481492	1.884017	-0.188118	H	-6.807510	4.223127	1.300416
C	-2.502835	4.617756	0.233765	H	-6.187991	3.271840	-0.079027
C	-4.052175	1.157427	1.015747	H	-0.610059	5.283248	0.877113
O	-4.297338	0.687948	2.103652	C	-0.044503	3.489659	2.888298
O	-4.702696	0.826424	-0.103878	C	0.673385	2.350724	3.303419
C	-3.598584	3.579940	0.322953	C	0.288384	4.732118	3.462701
H	-4.067125	3.461787	-0.662564	C	1.678489	2.448632	4.267714
H	-2.712757	5.498194	-0.375772	H	0.454761	1.381928	2.848587
C	-5.758676	-0.138570	0.015891	C	1.293693	4.829630	4.428670
H	-5.376629	-1.075686	0.445626	H	-0.258240	5.631447	3.169233
H	-6.562865	0.248214	0.659867	C	1.992945	3.688752	4.835666
H	-6.133701	-0.305464	-1.000112	H	2.227031	1.552821	4.569924
N	-4.718708	4.117585	1.197225	H	1.528843	5.802627	4.867478
C	-4.402796	4.249666	2.641221	H	2.782454	3.765718	5.587365



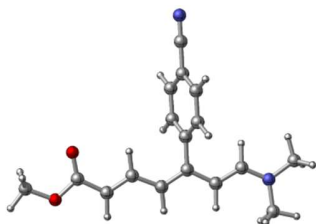
Zero-point correction=	0.332894 (Hartree/Particle)
Thermal correction to Energy=	0.352940
Thermal correction to Enthalpy=	0.353884
Thermal correction to Gibbs Free Energy=	0.282362
Sum of electronic and zero-point Energies=	-1286.132005
Sum of electronic and thermal Energies=	-1286.111959
Sum of electronic and thermal Enthalpies=	-1286.111015
Sum of electronic and thermal Free Energies=	-1286.182537

3b-CN

E(scf) = -917.939234334 a.u.

$\nu_{\min} = 24.62 \text{ cm}^{-1}$

C	0.185701	2.630576	-0.753421	H	2.062141	3.669819	-4.409342
C	-1.181832	2.480275	-0.882145	H	1.754284	5.306091	-3.763267
C	-2.040451	1.822030	0.050622	H	3.322194	4.928255	-4.531384
H	-1.593188	1.381252	0.947956	C	4.485580	4.421290	-2.359545
C	-3.390697	1.686075	-0.080266	H	5.133373	3.947760	-3.116616
H	-3.929204	2.093473	-0.939659	H	4.669961	5.509564	-2.382751
C	0.964884	3.259949	-1.784484	H	4.775833	4.043073	-1.370334
C	-4.174646	0.983896	0.936290	H	-1.648944	2.881911	-1.788630
O	-3.744399	0.469441	1.955627	C	0.881603	2.131869	0.473249
O	-5.492261	0.961137	0.618027	C	0.665063	2.744417	1.719580
C	2.310073	3.538808	-1.677742	C	1.766937	1.041753	0.397873
H	2.838112	3.278775	-0.756483	C	1.310515	2.283548	2.865311
H	0.423162	3.548819	-2.688010	H	-0.018499	3.592999	1.787290
C	-6.354923	0.300888	1.541864	C	2.415146	0.566816	1.535401
H	-6.075348	-0.758314	1.657850	H	1.942063	0.559122	-0.565744
H	-6.313750	0.778732	2.533583	C	2.190807	1.188714	2.778885
H	-7.368764	0.378701	1.129289	H	1.136066	2.767741	3.827828
N	3.086233	4.121224	-2.614671	H	3.093787	-0.285348	1.467310
C	2.526061	4.526760	-3.892097	C	2.859532	0.707820	3.954635



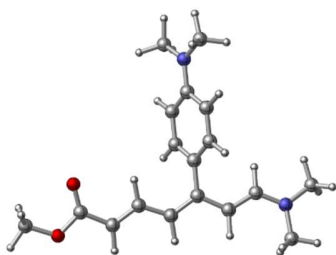
Zero-point correction= 0.315037 (Hartree/Particle)
 Thermal correction to Energy= 0.336667
 Thermal correction to Enthalpy= 0.337611
 Thermal correction to Gibbs Free Energy= 0.261096
 Sum of electronic and zero-point Energies= -917.624197
 Sum of electronic and thermal Energies= -917.602568
 Sum of electronic and thermal Enthalpies= -917.601624
 Sum of electronic and thermal Free Energies= -917.678138

3b-NMe₂

E(scf) = -959.643747074 a.u.

$\nu_{\min} = 24.82\text{cm}^{-1}$

C	0.209894	2.616378	-0.723447	H	2.028433	3.612953	-4.372030
C	-1.162244	2.474488	-0.864137	H	1.719448	5.292951	-3.851963
C	-2.029130	1.772109	0.023441	H	3.288307	4.857374	-4.589304
H	-1.584276	1.260107	0.882974	C	4.394185	4.669188	-2.327076
C	-3.384706	1.665810	-0.109323	H	5.112853	4.299106	-3.077126
H	-3.921027	2.149566	-0.929781	H	4.438741	5.773456	-2.326426
C	0.969217	3.254509	-1.770141	H	4.711944	4.311740	-1.338310
C	-4.173996	0.898761	0.849564	H	-1.625045	2.917161	-1.754190
O	-3.752383	0.292361	1.822320	C	0.909747	2.124630	0.496607
O	-5.496902	0.926779	0.540724	C	0.546530	2.565108	1.782138
C	2.292836	3.614357	-1.661824	C	1.962435	1.193884	0.418149
H	2.817753	3.431431	-0.720694	C	1.190031	2.108720	2.929331
H	0.423356	3.490848	-2.686861	H	-0.259054	3.296335	1.885171
C	-6.364241	0.209485	1.414350	C	2.611612	0.715468	1.552730
H	-6.107962	-0.861837	1.438096	H	2.271635	0.821145	-0.561667
H	-6.304500	0.599500	2.443087	C	2.246145	1.162064	2.851352
H	-7.380436	0.342667	1.021606	H	0.865852	2.498450	3.893310
N	3.053645	4.190878	-2.619479	H	3.406894	-0.017403	1.423112
C	2.492237	4.505529	-3.920549	N	2.886080	0.699835	3.980063



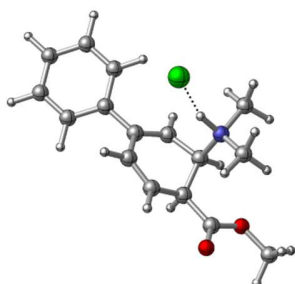
Zero-point correction=	0.388869 (Hartree/Particle)
Thermal correction to Energy=	0.413028
Thermal correction to Enthalpy=	0.413972
Thermal correction to Gibbs Free Energy=	0.332185
Sum of electronic and zero-point Energies=	-959.254878
Sum of electronic and thermal Energies=	-959.230719
Sum of electronic and thermal Enthalpies=	-959.229775
Sum of electronic and thermal Free Energies=	-959.311562

3b-OH-Cl

E(scf) = 31.48 a.u.

$\nu_{\min} = -1286.46292721 \text{ cm}^{-1}$

C	1.011009	1.182557	-0.015485	H	-2.378610	-2.077609	-1.880585
C	1.801852	0.018226	-0.452527	H	-1.725310	-1.263848	-3.348487
C	1.320004	-1.229685	-0.324429	H	-0.611320	-2.077929	-2.233695
H	1.887573	-2.113578	-0.619643	C	-2.577593	0.645305	-1.764960
C	-0.043214	-1.421031	0.283554	H	-2.653432	0.879266	-2.833624
H	0.070688	-1.290423	1.381687	H	-3.476605	0.123333	-1.410110
C	-0.311745	1.035248	0.237076	H	-2.443855	1.582780	-1.213916
C	-0.583701	-2.839644	0.167758	H	2.791753	0.196597	-0.876582
O	0.071625	-3.799671	-0.160513	C	1.683238	2.499346	0.103733
O	-1.870811	-2.903027	0.527638	C	1.089035	3.649420	-0.447311
C	-0.995601	-0.276155	-0.088428	C	2.930427	2.619815	0.742971
H	-1.932303	-0.400101	0.469005	C	1.714006	4.893774	-0.334735
H	-0.916661	1.881250	0.567052	H	0.158293	3.545038	-1.008147
C	-2.483064	-4.201855	0.514951	C	3.551940	3.865933	0.859539
H	-2.457113	-4.627796	-0.499068	H	3.408468	1.732341	1.165923
H	-1.957474	-4.880905	1.201919	C	2.943697	5.007149	0.323983
H	-3.518648	-4.052129	0.840676	H	1.245595	5.777556	-0.775550
N	-1.381038	-0.217117	-1.570729	H	4.515111	3.946485	1.369897
C	-1.541243	-1.502646	-2.293326	H	3.432875	5.980786	0.409793



Zero-point correction=	0.333022 (Hartree/Particle)
Thermal correction to Energy=	0.353024
Thermal correction to Enthalpy=	0.353968
Thermal correction to Gibbs Free Energy=	0.283172
Sum of electronic and zero-point Energies=	-1286.129905
Sum of electronic and thermal Energies=	-1286.109903
Sum of electronic and thermal Enthalpies=	-1286.108959
Sum of electronic and thermal Free Energies=	-1286.179755

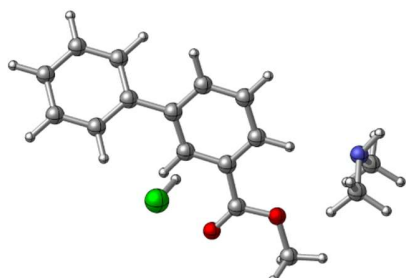
4a

E(scf) = -1286.47968161 a.u.

$\nu_{\min} = 15.31 \text{ cm}^{-1}$

C	-1.256223	4.749386	2.080816	C	-7.302272	4.126061	1.464088
C	-0.744132	3.493826	2.464015	H	-6.895158	3.190676	1.880717
C	-1.603699	2.384756	2.398778	H	-7.303877	4.876318	2.270439
H	-1.257871	1.398102	2.711601	H	-8.358872	3.933868	1.172331
C	-2.928657	2.514566	1.948373	C	-6.486292	3.693328	-0.787727
H	-1.080946	1.982612	0.261665	H	-6.024802	2.728040	-0.524001
C	-2.575009	4.881507	1.641095	H	-7.509234	3.484186	-1.172736
C	-3.753396	1.269644	1.887057	H	-5.896989	4.130291	-1.609215
O	-3.339275	0.164065	2.166292	H	-0.604488	5.625712	2.105012
O	-5.012678	1.494302	1.480814	C	0.665456	3.338241	2.909122
C	-3.421897	3.771985	1.565353	C	1.426300	2.224284	2.504967
H	-4.446585	3.902135	1.205035	C	1.273552	4.301326	3.736175
H	-2.949310	5.862399	1.337607	C	2.752203	2.077070	2.919902
C	-5.867285	0.350168	1.379178	H	0.987110	1.485822	1.830757
H	-5.459848	-0.374782	0.658820	C	2.598951	4.151945	4.152275
H	-5.973480	-0.142301	2.357264	H	0.695923	5.164684	4.075121
H	-6.837433	0.726403	1.034144	C	3.343367	3.038747	3.746632
N	-6.459160	4.575437	0.367944	H	3.329055	1.210134	2.587836

H 3.050295 4.906008 4.802138 H 4.380291 2.922452 4.071641



Zero-point correction= 0.326046 (Hartree/Particle)
 Thermal correction to Energy= 0.349029
 Thermal correction to Enthalpy= 0.349973
 Thermal correction to Gibbs Free Energy= 0.268850
 Sum of electronic and zero-point Energies= -1286.153636
 Sum of electronic and thermal Energies= -1286.130653
 Sum of electronic and thermal Enthalpies= -1286.129708
 Sum of electronic and thermal Free Energies= -1286.210832

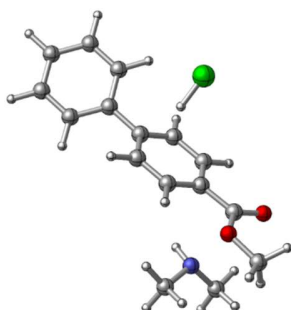
4b

E(scf) = -1286.48029470 a.u.

$\nu_{\min} = 18.56 \text{ cm}^{-1}$

C	1.132613	1.193749	0.259997	C	-2.533643	-1.726717	-3.755208
C	1.591007	0.082162	-0.473992	H	-3.315999	-2.460414	-3.495312
C	0.774365	-1.026882	-0.677695	H	-2.861372	-1.215706	-4.688166
H	1.132272	-1.886432	-1.247118	H	-1.615248	-2.292395	-3.976999
C	-0.527850	-1.059288	-0.158219	C	-3.454203	-0.049612	-2.238126
H	1.036006	-0.271263	2.322907	H	-3.881016	0.581917	-3.049213
C	-0.178988	1.153584	0.776278	H	-4.258802	-0.716633	-1.883777
C	-1.362039	-2.271851	-0.407474	H	-3.181281	0.610297	-1.399743
O	-0.974464	-3.258192	-0.998733	H	2.599757	0.092392	-0.891794
O	-2.579078	-2.181493	0.153194	C	2.020369	2.353520	0.524889
C	-0.998637	0.041451	0.573379	C	1.531367	3.672070	0.464314
H	-2.005844	0.019626	0.989845	C	3.372525	2.152901	0.862946
H	-0.550759	1.992924	1.368001	C	2.371582	4.757688	0.723955
C	-3.471107	-3.267585	-0.093512	H	0.488327	3.848480	0.190581
H	-3.670014	-3.362507	-1.171888	C	4.210894	3.238886	1.126046
H	-3.049353	-4.216084	0.272183	H	3.757985	1.134872	0.953560
H	-4.398951	-3.032314	0.441836	C	3.714576	4.545342	1.055046
N	-2.306363	-0.837172	-2.634921	H	1.976622	5.774942	0.662229

H 5.255212 3.063244 1.396485 H 4.371079 5.394736 1.259731



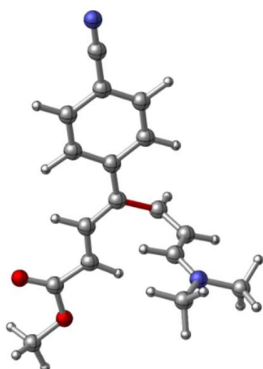
Zero-point correction= 0.325271 (Hartree/Particle)
 Thermal correction to Energy= 0.348527
 Thermal correction to Enthalpy= 0.349472
 Thermal correction to Gibbs Free Energy= 0.267233
 Sum of electronic and zero-point Energies= -1286.155024
 Sum of electronic and thermal Energies= -1286.131767
 Sum of electronic and thermal Enthalpies= -1286.130823
 Sum of electronic and thermal Free Energies= -1286.213062

TS-3a-CN-r

E(scf) = -917.896137009 a.u.

$\nu_{\min} = -347.98\text{cm}^{-1}$

C	-0.291692	3.292653	-0.428516	C	2.987182	2.706835	2.269227
C	-1.687240	3.422865	0.059912	H	3.598014	2.670730	3.177511
C	-2.417743	2.232063	0.206587	H	3.177927	1.804401	1.670689
H	-0.109374	3.337087	-1.513321	H	3.261036	3.597540	1.688158
H	-3.470400	2.317592	0.495666	C	1.262122	2.587408	4.072582
C	-1.970409	0.928105	0.041933	H	1.645873	1.611232	4.404385
H	-0.939698	0.697822	-0.233937	H	1.753924	3.381056	4.654089
C	0.798603	3.085756	0.359571	H	0.178527	2.629945	4.232122
C	-2.865148	-0.184153	0.245305	C	-2.212299	4.743529	0.298338
O	-4.049550	-0.141210	0.566569	C	-3.550079	4.983348	0.743884
O	-2.236741	-1.385777	0.040842	C	-1.405062	5.906756	0.099234
C	0.620905	2.947606	1.772851	C	-4.030170	6.259713	0.971040
H	-0.406206	2.985866	2.150042	H	-4.222226	4.142266	0.918433
H	1.790626	2.991717	-0.085006	C	-1.882578	7.187114	0.325363
C	-3.034937	-2.547652	0.217874	H	-0.373053	5.792251	-0.239790
H	-3.428438	-2.615422	1.245675	C	-3.208431	7.396720	0.768612
H	-3.893587	-2.557421	-0.473632	H	-5.058853	6.395359	1.313565
H	-2.384377	-3.408619	0.012876	H	-1.227710	8.045854	0.159058
N	1.567700	2.766957	2.650259	C	-3.703335	8.711732	1.005951



Zero-point correction=	0.313888 (Hartree/Particle)
Thermal correction to Energy=	0.334971
Thermal correction to Enthalpy=	0.335915
Thermal correction to Gibbs Free Energy=	0.261130
Sum of electronic and zero-point Energies=	-917.582249
Sum of electronic and thermal Energies=	-917.561166
Sum of electronic and thermal Enthalpies=	-917.560222
Sum of electronic and thermal Free Energies=	-917.635007

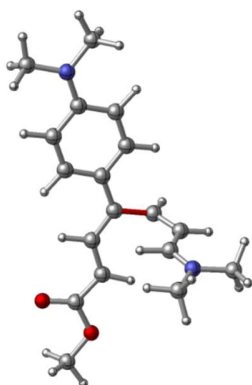
TS-3a-NMe₂-r

E(scf) = -959.586084050 a.u.

$\nu_{\min} = -704.70\text{cm}^{-1}$

C	-0.236286	3.392531	-0.395582	H	-2.215536	-3.353484	0.057720
C	-1.643163	3.495060	0.063439	N	1.491244	2.538851	2.685597
C	-2.350990	2.308058	0.188946	C	2.927284	2.541855	2.374894
H	-0.016502	3.514199	-1.468318	H	3.494466	2.462289	3.308854
H	-3.409549	2.378004	0.463824	H	3.174910	1.685853	1.729775
C	-1.877613	0.990478	0.042748	H	3.204355	3.474884	1.866835
H	-0.838564	0.778278	-0.215026	C	1.116478	2.164102	4.051132
C	0.826404	3.116841	0.410604	H	1.505205	1.158749	4.272147
C	-2.748331	-0.124080	0.239000	H	1.555537	2.879997	4.761646
O	-3.945138	-0.113105	0.539488	H	0.025041	2.164061	4.153749
O	-2.093364	-1.330164	0.060589	C	-2.179808	4.836064	0.321391
C	0.584213	2.814545	1.787554	C	-3.488161	5.068310	0.812540
H	-0.460888	2.795890	2.111560	C	-1.411754	6.001770	0.088438
H	1.835484	3.055676	-0.001233	C	-3.984333	6.346151	1.052697
C	-2.878269	-2.495534	0.239921	H	-4.147325	4.222088	1.018610
H	-3.290642	-2.559939	1.261531	C	-1.895091	7.288891	0.328745
H	-3.727513	-2.530794	-0.463686	H	-0.393802	5.907783	-0.300837

C	-3.198849	7.507109	0.832744	H	-1.236341	8.130678	0.115329
H	-5.004217	6.434388	1.427183	N	-3.683629	8.785070	1.103247



Zero-point correction=	0.386698 (Hartree/Particle)
Thermal correction to Energy=	0.410541
Thermal correction to Enthalpy=	0.411485
Thermal correction to Gibbs Free Energy=	0.329982
Sum of electronic and zero-point Energies=	-959.199386
Sum of electronic and thermal Energies=	-959.175543
Sum of electronic and thermal Enthalpies=	-959.174599
Sum of electronic and thermal Free Energies=	-959.256102

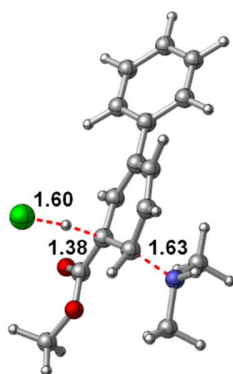
TS-3a-OH-Cl

E(scf) = -1286.43540909a.u.

$\nu_{\min} = -885.32\text{cm}^{-1}$

C	-1.450874	4.494621	1.026714	H	-2.678819	5.322503	-0.504939
C	-1.194426	3.426580	1.984129	C	-5.750828	-0.134073	0.042769
C	-2.034968	2.347064	1.942994	H	-5.121557	-0.953189	-0.337693
H	-1.885773	1.489523	2.601792	H	-6.180901	-0.437485	1.009087
C	-3.107752	2.239525	0.967320	H	-6.549721	0.091669	-0.674200
H	-2.432613	1.817224	-0.160911	N	-4.834652	4.222485	1.194707
C	-2.549844	4.528121	0.235089	C	-4.596274	4.216520	2.663345
C	-3.953123	1.030600	1.052307	H	-4.652535	3.183488	3.025245
O	-3.728095	0.061885	1.751850	H	-3.599700	4.625084	2.862705
O	-4.984223	1.064420	0.176076	H	-5.363372	4.827916	3.155955
C	-3.634537	3.506021	0.361588	C	-6.204083	3.751653	0.845363
H	-4.126384	3.302072	-0.597541	H	-6.333183	2.728059	1.206945

H	-6.939667	4.418723	1.313691	H	0.361621	1.393950	2.961020
H	-6.321247	3.769695	-0.244793	C	1.434605	4.864612	4.329036
H	-0.698775	5.279688	0.910357	H	-0.157706	5.679534	3.131493
C	-0.054042	3.521520	2.926878	C	2.107997	3.713687	4.750783
C	0.642398	2.372561	3.357030	H	2.228537	1.559307	4.570680
C	0.368198	4.769373	3.430306	H	1.736082	5.845341	4.706778
C	1.703774	2.466465	4.259165	H	2.942733	3.787117	5.452373



Zero-point correction=	0.328032 (Hartree/Particle)
Thermal correction to Energy=	0.348040
Thermal correction to Enthalpy=	0.348984
Thermal correction to Gibbs Free Energy=	0.277889
Sum of electronic and zero-point Energies=	-1286.107377
Sum of electronic and thermal Energies=	-1286.087369
Sum of electronic and thermal Enthalpies=	-1286.086425
Sum of electronic and thermal Free Energies=	-1286.157520

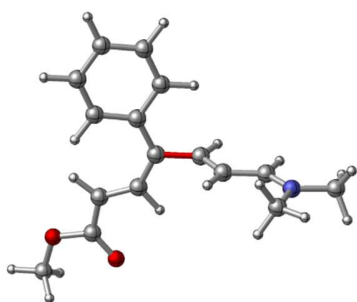
TS-3a-r-conf1

E(scf) = -825.700714105 a.u.

$\nu_{\min} = -691.73\text{cm}^{-1}$

C	-0.218775	3.261164	-0.197115	O	-5.504354	0.339477	-0.008659
C	-1.663779	3.387888	0.119614	C	2.108962	2.864214	0.302364
C	-2.380893	2.192648	-0.002102	H	2.331374	2.968384	-0.764678
H	0.110283	3.366681	-1.246325	H	0.482146	2.897271	1.774569
H	-1.759297	1.319569	-0.247801	C	-6.004812	-0.974681	-0.185217
C	-3.733008	1.847412	0.101247	H	-5.742480	-1.382380	-1.176154
H	-4.529156	2.563573	0.291529	H	-5.609957	-1.668405	0.576535
C	0.752135	3.003103	0.721945	H	-7.097990	-0.910399	-0.091683
C	-4.134698	0.485267	-0.098433	N	3.129001	2.617200	1.078571
O	-3.423961	-0.495901	-0.323568	C	2.975531	2.455221	2.532591

H	2.532249	3.361015	2.968889	C	-1.299865	5.861110	0.268602
H	2.331183	1.591654	2.749852	C	-3.861704	6.290318	1.254903
H	3.961967	2.288210	2.977691	H	-4.124807	4.168858	1.153220
C	4.485012	2.482474	0.539832	C	-1.725355	7.154811	0.566199
H	5.135466	3.244140	0.994750	H	-0.285144	5.724647	-0.114906
H	4.877343	1.484797	0.786259	C	-3.015286	7.389244	1.060351
H	4.471930	2.613042	-0.548673	H	-4.869046	6.443123	1.654213
C	-2.144149	4.726427	0.442325	H	-1.039477	7.992642	0.408046
C	-3.443654	4.993085	0.956170	H	-3.350367	8.403036	1.292990



Zero-point correction= 0.315181 (Hartree/Particle)

Thermal correction to Energy= 0.334363

Thermal correction to Enthalpy= 0.335307

Thermal correction to Gibbs Free Energy= 0.265268

Sum of electronic and zero-point Energies= -825.385533

Sum of electronic and thermal Energies= -825.366352

Sum of electronic and thermal Enthalpies= -825.365407

Sum of electronic and thermal Free Energies= -825.435446

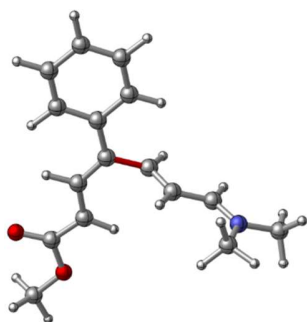
TS-3a-r-conf2

E(scf) = -825.706538428a.u.

$\nu_{\min} = -736.33\text{cm}^{-1}$

C	-0.212193	3.156534	-0.117305	O	-2.229624	-0.929883	2.156554
C	-1.565908	3.520073	0.348265	C	2.173484	2.862275	0.089853
C	-2.295548	2.515447	0.983486	H	2.184526	2.446284	-0.922970
H	-0.100725	2.717312	-1.124626	H	0.860834	3.711365	1.629623
H	-3.319567	2.757922	1.288787	C	-3.049182	-1.891990	2.798156
C	-1.902583	1.207837	1.287428	H	-3.367293	-1.556236	3.799858
H	-0.903484	0.835474	1.050500	H	-3.960110	-2.108108	2.214366
C	0.921368	3.287785	0.625237	H	-2.447126	-2.806827	2.891351
C	-2.803418	0.307678	1.940415	N	3.326126	2.919301	0.699744
O	-3.961523	0.522926	2.302747	C	3.455147	3.452203	2.064851

H	3.141465	4.505308	2.090022	C	-1.263571	5.795289	-0.665721
H	2.833605	2.868658	2.758192	C	-3.810586	6.586253	0.119856
H	4.502602	3.381828	2.376336	H	-4.023644	4.635341	0.975358
C	4.557291	2.453998	0.055749	C	-1.723244	7.077821	-0.970539
H	5.273962	3.286475	-0.003363	H	-0.256122	5.512569	-0.982755
H	4.998894	1.644981	0.656248	C	-3.001950	7.493287	-0.582746
H	4.339137	2.085153	-0.953346	H	-4.814531	6.884951	0.436724
C	-2.063356	4.856897	0.044095	H	-1.069195	7.762004	-1.519836
C	-3.359465	5.304822	0.425470	H	-3.361940	8.497453	-0.819405



Zero-point correction=	0.314826 (Hartree/Particle)
Thermal correction to Energy=	0.334121
Thermal correction to Enthalpy=	0.335065
Thermal correction to Gibbs Free Energy=	0.264539
Sum of electronic and zero-point Energies=	-825.391712
Sum of electronic and thermal Energies=	-825.372418
Sum of electronic and thermal Enthalpies=	-825.371474
Sum of electronic and thermal Free Energies=	-825.442000

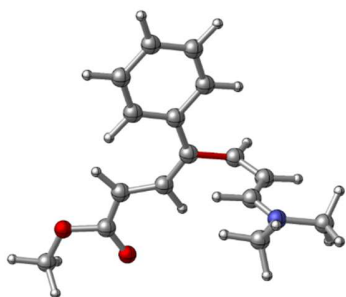
TS-3a-r-conf3

E(scf) = -825.702957391 a.u.

$\nu_{\min} = -685.20 \text{ cm}^{-1}$

C	-0.076305	3.719483	-0.369196	C	-3.643279	0.503490	-0.205740
C	-1.500912	3.654439	0.061342	O	-2.844632	-0.371015	-0.544314
C	-2.090254	2.394846	-0.103198	O	-4.976763	0.193707	-0.037381
H	0.152242	3.904039	-1.431472	C	0.801700	3.331417	1.841852
H	-1.394669	1.617941	-0.451533	H	-0.235550	3.262793	2.185632
C	-3.383325	1.889155	0.062629	H	2.015543	3.618268	0.037156
H	-4.239649	2.493880	0.352069	C	-5.338324	-1.156153	-0.276003
C	1.005279	3.562147	0.446265	H	-5.115965	-1.461357	-1.312522

H	-4.803988	-1.847285	0.397689	C	-2.100345	4.898877	0.531630
H	-6.419928	-1.228782	-0.095445	C	-3.378971	4.970241	1.151608
N	1.735278	3.192663	2.741673	C	-1.399454	6.133752	0.411119
C	3.164414	3.263343	2.401032	C	-3.910188	6.180028	1.600219
H	3.423577	2.462272	1.694444	H	-3.951527	4.060298	1.312937
H	3.397503	4.238404	1.951081	C	-1.939370	7.339741	0.855399
H	3.755198	3.139996	3.314924	H	-0.407172	6.147498	-0.047011
C	1.405610	2.954187	4.149638	C	-3.205113	7.381351	1.454570
H	1.852094	2.001625	4.471270	H	-4.894531	6.180958	2.078320
H	1.819395	3.768008	4.763442	H	-1.362243	8.261069	0.731320
H	0.317834	2.912940	4.278416	H	-3.628874	8.326079	1.803927



Zero-point correction=	0.315119 (Hartree/Particle)
Thermal correction to Energy=	0.334312
Thermal correction to Enthalpy=	0.335256
Thermal correction to Gibbs Free Energy=	0.265154
Sum of electronic and zero-point Energies=	-825.387838
Sum of electronic and thermal Energies=	-825.368645
Sum of electronic and thermal Enthalpies=	-825.367701
Sum of electronic and thermal Free Energies=	-825.437804

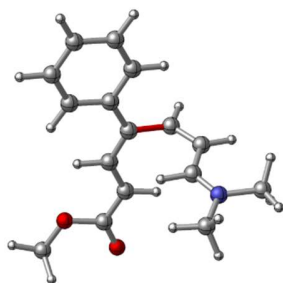
TS-3a-r-conf4

E(scf) = -825.708282959 a.u.

$\nu_{\min} = -497.22\text{cm}^{-1}$

C	-0.308194	3.339176	-0.434531	C	0.771511	3.089006	0.357050
C	-1.700721	3.497695	0.050770	C	-2.837022	-0.147587	0.282920
C	-2.448272	2.331371	0.213778	O	-2.477814	-1.321578	0.193783
H	-0.115869	3.393325	-1.517881	O	-4.145795	0.150040	0.605433
H	-3.499096	2.451150	0.492729	C	0.568478	2.892909	1.759045
C	-2.010822	1.006793	0.086712	H	-0.464921	2.931758	2.118213
H	-0.974374	0.774790	-0.167488	H	1.765937	2.981076	-0.079498

C	-5.002168	-0.957978	0.825144	H	0.076770	2.449298	4.188442
H	-5.079215	-1.597568	-0.070145	C	-2.198929	4.850929	0.274847
H	-4.648165	-1.588818	1.657920	C	-3.511102	5.123025	0.753085
H	-5.991312	-0.546374	1.069712	C	-1.379693	5.985410	0.021114
N	1.497504	2.652921	2.643371	C	-3.960934	6.425399	0.956346
C	2.921155	2.585695	2.282961	H	-4.189082	4.296921	0.976275
H	3.517864	2.515523	3.198853	C	-1.835803	7.288169	0.229939
H	3.110502	1.698418	1.661289	H	-0.360455	5.841032	-0.347208
H	3.215967	3.488626	1.731904	C	-3.132120	7.528212	0.699271
C	1.162590	2.399022	4.046993	H	-4.978308	6.584074	1.326815
H	1.524362	1.399577	4.331353	H	-1.166277	8.127730	0.019397
H	1.653774	3.150537	4.682686	H	-3.490089	8.547598	0.862479



Zero-point correction=	0.314631 (Hartree/Particle)
Thermal correction to Energy=	0.334012
Thermal correction to Enthalpy=	0.334956
Thermal correction to Gibbs Free Energy=	0.263534
Sum of electronic and zero-point Energies=	-825.393652
Sum of electronic and thermal Energies=	-825.374271
Sum of electronic and thermal Enthalpies=	-825.373327
Sum of electronic and thermal Free Energies=	-825.444749

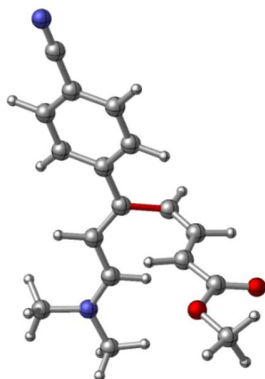
TS-3b-CN-r

E(scf) = -917.884245502 a.u.

$\nu_{\min} = -669.7\text{cm}^{-1}$

C	-1.494279	4.874621	0.938251	C	-2.828391	5.217791	0.963948
C	-1.038761	3.573569	0.391315	C	-1.597395	0.961029	3.060380
C	-1.075837	2.418041	1.135439	O	-1.199657	-0.114269	2.601466
H	-0.693005	1.506665	0.659097	O	-2.141327	1.003947	4.335451
C	-1.588561	2.242915	2.440624	C	-3.801130	4.261736	0.560343
H	-1.992994	3.085998	3.005358	H	-3.431194	3.282465	0.243411

H	-3.153946	6.169377	1.385555	H	-5.440044	2.444411	-0.023741
C	-2.190575	-0.228696	5.029845	H	-0.656832	3.579602	-0.633647
H	-2.801573	-0.977713	4.497076	C	-0.483977	5.802940	1.496959
H	-1.185495	-0.662091	5.171360	C	0.715779	5.283742	2.029106
H	-2.640583	-0.020807	6.011272	C	-0.669894	7.202750	1.496492
N	-5.099084	4.441436	0.556641	C	1.679098	6.123299	2.575222
C	-5.715588	5.714213	0.947836	H	0.868987	4.203895	2.020779
H	-6.775565	5.698035	0.670312	C	0.300377	8.054383	2.014331
H	-5.632012	5.857915	2.035847	H	-1.569315	7.637430	1.057388
H	-5.225759	6.550437	0.431321	C	1.480507	7.519416	2.565743
C	-6.011527	3.349260	0.214233	H	2.592006	5.706586	3.004157
H	-6.675881	3.146455	1.068059	H	0.151254	9.135282	1.991351
H	-6.625142	3.637852	-0.652286	C	2.480790	8.393916	3.106724



Zero-point correction=	0.312797 (Hartree/Particle)
Thermal correction to Energy=	0.334049
Thermal correction to Enthalpy=	0.334993
Thermal correction to Gibbs Free Energy=	0.259484
Sum of electronic and zero-point Energies=	-917.571449
Sum of electronic and thermal Energies=	-917.550196
Sum of electronic and thermal Enthalpies=	-917.549252
Sum of electronic and thermal Free Energies=	-917.624762

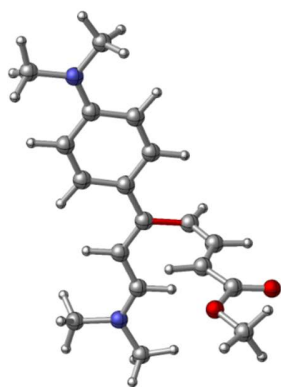
TS-3b-NMe₂-r

E(scf) = -959.598007767 a.u.

$\nu_{\min} = -415.07 \text{ cm}^{-1}$

C	-1.404495	4.861013	0.947500	C	-1.300937	2.302805	2.632971
C	-0.984037	3.519787	0.457288	H	-1.656972	3.172682	3.190439
C	-0.941238	2.412414	1.268824	C	-2.763027	5.189881	0.980830
H	-0.607748	1.474422	0.805624	C	-1.220813	1.062114	3.316433

O	-0.855250	-0.038195	2.883566	H	-6.609950	3.114634	1.247510
O	-1.626784	1.169547	4.644719	H	-6.600475	3.575066	-0.480967
C	-3.735181	4.228743	0.662051	H	-5.395899	2.404083	0.141083
H	-3.381528	3.231377	0.386079	H	-0.712292	3.446485	-0.600460
H	-3.086433	6.178461	1.305392	C	-0.389721	5.800588	1.395466
C	-1.583364	-0.023193	5.402029	C	0.982718	5.443964	1.344426
H	-2.234742	-0.807703	4.978397	C	-0.679247	7.095884	1.904869
H	-0.562910	-0.440636	5.460577	C	1.988938	6.294086	1.762958
H	-1.930904	0.230736	6.414314	H	1.239395	4.455038	0.960616
N	-5.045623	4.408775	0.675727	C	0.310072	7.962294	2.325436
C	-5.638518	5.699164	1.025527	H	-1.712080	7.438732	1.982244
H	-5.405517	5.962482	2.069233	C	1.689560	7.592800	2.270497
H	-5.254573	6.491384	0.365393	H	3.020192	5.951385	1.696639
H	-6.726988	5.640623	0.910586	H	0.016508	8.938811	2.706815
C	-5.963190	3.312476	0.378048	N	2.670758	8.443433	2.684474



Zero-point correction=	0.387196 (Hartree/Particle)
Thermal correction to Energy=	0.410895
Thermal correction to Enthalpy=	0.411840
Thermal correction to Gibbs Free Energy=	0.331357
Sum of electronic and zero-point Energies=	-959.210812
Sum of electronic and thermal Energies=	-959.187112
Sum of electronic and thermal Enthalpies=	-959.186168
Sum of electronic and thermal Free Energies=	-959.266650

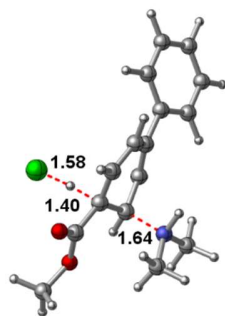
TS-3b-OH-Cl

E(scf) = -1286.43544267 a.u.

$\nu_{\min} = -915.45\text{cm}^{-1}$

C	-1.682883	4.294776	0.162714	C	-1.016430	3.118641	-0.385518
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C	-1.660245	1.918433	-0.386379	H	-5.157071	2.455062	-3.261238
H	-1.150353	1.000689	-0.688467	H	-4.101953	1.374152	-2.303203
C	-3.023724	1.813281	0.110296	C	-5.205514	4.514875	-1.618312
H	-2.829201	1.811840	1.494099	H	-5.404836	4.763251	-2.668654
C	-3.024254	4.249637	0.421118	H	-6.144959	4.257868	-1.111701
C	-3.668286	0.488326	0.072600	H	-4.736091	5.371098	-1.121553
O	-3.101615	-0.563543	-0.156552	H	0.016987	3.198685	-0.726329
O	-4.979766	0.544788	0.406933	C	-0.880620	5.503241	0.487659
C	-3.829557	3.064010	-0.001479	C	-1.409851	6.796428	0.310373
H	-4.788519	2.982094	0.522311	C	0.428518	5.383381	0.993532
H	-3.525693	5.076377	0.925835	C	-0.661220	7.929773	0.636389
C	-5.659763	-0.705429	0.529111	H	-2.411785	6.913541	-0.108733
H	-5.629911	-1.264171	-0.418894	C	1.176574	6.516703	1.322577
H	-5.200077	-1.322782	1.315919	H	0.855588	4.391010	1.154172
H	-6.696835	-0.466277	0.794744	C	0.635364	7.794680	1.145243
N	-4.293440	3.343549	-1.545116	H	-1.089352	8.923910	0.484048
C	-4.860857	2.161473	-2.245703	H	2.186460	6.400246	1.724150
H	-5.728826	1.799866	-1.683806	H	1.222246	8.681093	1.398845



Zero-point correction= 0.327642 (Hartree/Particle)
 Thermal correction to Energy= 0.347737
 Thermal correction to Enthalpy= 0.348681
 Thermal correction to Gibbs Free Energy= 0.277272
 Sum of electronic and zero-point Energies= -1286.107801
 Sum of electronic and thermal Energies= -1286.087706

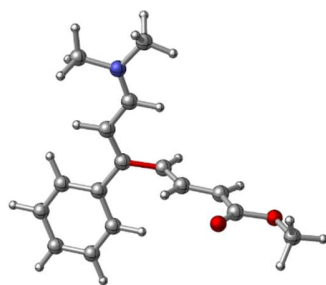
Sum of electronic and thermal Enthalpies= -1286.086761
 Sum of electronic and thermal Free Energies= -1286.158171

TS-3b-r-conf1

E(scf) = -825.704568836 a.u.

$\nu_{\min} = -996.86 \text{ cm}^{-1}$

C	0.393082	2.657997	-0.556041	H	3.237376	4.169979	-3.230698
C	-1.075527	2.829134	-0.666143	H	3.179383	2.486837	-3.845552
C	-1.938498	1.817752	-1.017553	H	3.169821	3.860682	-4.988431
H	-1.487882	0.841931	-1.251539	C	0.678157	3.893596	-5.230248
C	-3.344957	1.844353	-1.134517	H	0.987135	4.897802	-5.558291
H	-3.907956	2.757149	-0.921063	H	0.954305	3.166480	-6.009078
C	1.222700	2.907041	-1.638629	H	-0.408680	3.875248	-5.086543
C	-4.065382	0.690155	-1.540426	H	-1.455248	3.825869	-0.406384
O	-3.627449	-0.428965	-1.836229	C	0.976627	2.236112	0.738800
O	-5.436492	0.920284	-1.589560	C	0.133516	1.696468	1.735585
C	0.675499	3.281116	-2.888285	C	2.356170	2.357400	1.033484
H	-0.415081	3.338943	-2.955891	C	0.647909	1.269593	2.960164
H	2.301888	2.784942	-1.552690	H	-0.932840	1.609686	1.525291
C	-6.234271	-0.178326	-1.984144	C	2.865392	1.947426	2.263105
H	-5.987488	-0.525029	-3.003031	H	3.040635	2.799037	0.307835
H	-6.116275	-1.041134	-1.305635	C	2.014410	1.395257	3.230394
H	-7.279253	0.163926	-1.959986	H	-0.022434	0.842816	3.710050
N	1.355451	3.553947	-3.978404	H	3.931492	2.061991	2.473284
C	2.821484	3.514394	-4.009009	H	2.417023	1.071827	4.193580



Zero-point correction= 0.314559 (Hartree/Particle)

Thermal correction to Energy= 0.333814

Thermal correction to Enthalpy= 0.334758

Thermal correction to Gibbs Free Energy= 0.264384

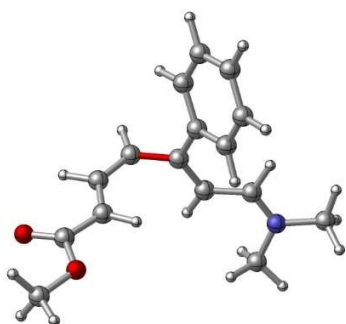
Sum of electronic and zero-point Energies= -825.390010
 Sum of electronic and thermal Energies= -825.370755
 Sum of electronic and thermal Enthalpies= -825.369811
 Sum of electronic and thermal Free Energies= -825.440185

TS-3b-r-conf2

E(scf) = -825.706538428 a.u.

$\nu_{\min} = -736.33 \text{ cm}^{-1}$

C	-0.212193	3.156534	-0.117305	C	3.455147	3.452203	2.064851
C	-1.565908	3.520073	0.348265	H	3.141465	4.505308	2.090022
C	-2.295548	2.515447	0.983486	H	2.833605	2.868658	2.758192
H	-0.100725	2.717312	-1.124626	H	4.502602	3.381828	2.376336
H	-3.319567	2.757922	1.288787	C	4.557291	2.453998	0.055749
C	-1.902583	1.207837	1.287428	H	5.273962	3.286475	-0.003363
H	-0.903484	0.835474	1.050500	H	4.998894	1.644981	0.656248
C	0.921368	3.287785	0.625237	H	4.339137	2.085153	-0.953346
C	-2.803418	0.307678	1.940415	C	-2.063356	4.856897	0.044095
O	-3.961523	0.522926	2.302747	C	-3.359465	5.304822	0.425470
O	-2.229624	-0.929883	2.156554	C	-1.263571	5.795289	-0.665721
C	2.173484	2.862275	0.089853	C	-3.810586	6.586253	0.119856
H	2.184526	2.446284	-0.922970	H	-4.023644	4.635341	0.975358
H	0.860834	3.711365	1.629623	C	-1.723244	7.077821	-0.970539
C	-3.049182	-1.891990	2.798156	H	-0.256122	5.512569	-0.982755
H	-3.367293	-1.556236	3.799858	C	-3.001950	7.493287	-0.582746
H	-3.960110	-2.108108	2.214366	H	-4.814531	6.884951	0.436724
H	-2.447126	-2.806827	2.891351	H	-1.069195	7.762004	-1.519836
N	3.326126	2.919301	0.699744	H	-3.361940	8.497453	-0.819405



Zero-point correction= 0.314826 (Hartree/Particle)
 Thermal correction to Energy= 0.334121
 Thermal correction to Enthalpy= 0.335065

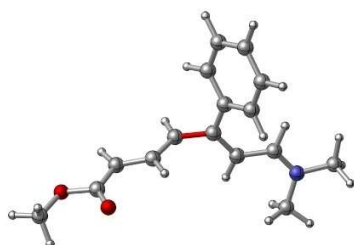
Thermal correction to Gibbs Free Energy= 0.264539
 Sum of electronic and zero-point Energies= -825.391712
 Sum of electronic and thermal Energies= -825.372418
 Sum of electronic and thermal Enthalpies= -825.371474
 Sum of electronic and thermal Free Energies= -825.442000

TS-3b-r-conf3

E(scf) = -825.696465517 a.u.

$\nu_{\min} = -1251.88\text{cm}^{-1}$

C	0.337279	2.999965	0.070093	H	1.080722	2.778858	-3.905328
C	-1.104091	3.149053	0.375464	H	1.168032	4.569299	-3.952486
C	-2.016556	2.140739	0.178494	H	2.376839	3.587779	-4.831698
H	-1.628184	1.193702	-0.224475	C	4.056649	3.888756	-2.989395
C	-3.409541	2.136318	0.411694	H	4.463889	3.119666	-3.662597
H	-3.914159	3.020136	0.811762	H	4.175938	4.874513	-3.464289
C	0.798910	3.307081	-1.196309	H	4.607005	3.874191	-2.041148
C	-4.191962	0.987590	0.127396	H	-1.411234	4.118909	0.789237
O	-3.826453	-0.104384	-0.327807	C	1.235389	2.510338	1.140004
O	-5.538618	1.184941	0.422189	C	1.052104	2.960358	2.466268
C	2.170569	3.436387	-1.539468	C	2.241909	1.552589	0.888215
H	2.920171	3.425879	-0.743673	C	1.886511	2.515238	3.488499
H	0.044956	3.549499	-1.946969	H	0.253302	3.672910	2.679278
C	-6.392396	0.086730	0.171751	C	3.057225	1.084604	1.922706
H	-6.376026	-0.218127	-0.889318	H	2.348904	1.131426	-0.113599
H	-6.116619	-0.798412	0.771636	C	2.891119	1.573412	3.221125
H	-7.409176	0.406787	0.443183	H	1.748023	2.892801	4.504473
N	2.636064	3.630073	-2.751001	H	3.816109	0.326902	1.713283
C	1.759788	3.641452	-3.927717	H	3.529922	1.209883	4.029781



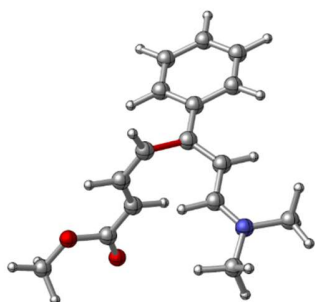
Zero-point correction=	0.314281 (Hartree/Particle)
Thermal correction to Energy=	0.333610
Thermal correction to Enthalpy=	0.334554
Thermal correction to Gibbs Free Energy=	0.264018
Sum of electronic and zero-point Energies=	-825.382185
Sum of electronic and thermal Energies=	-825.362855
Sum of electronic and thermal Enthalpies=	-825.361911
Sum of electronic and thermal Free Energies=	-825.432448

TS-3b-r-conf4

E(scf) = -825.706768383 a.u.

$\nu_{\min} = -596.15 \text{ cm}^{-1}$

C	-1.380630	4.882008	0.933473	H	-5.197073	6.496009	0.593556
C	-0.950422	3.581567	0.360638	H	-6.691377	5.610085	1.005907
C	-0.884295	2.429183	1.108258	H	-5.420163	5.829978	2.243304
H	-0.535131	1.530191	0.587498	C	-5.914384	3.292670	0.441164
C	-1.252805	2.258102	2.463635	H	-6.527487	3.066022	1.326932
H	-1.622976	3.107828	3.043742	H	-6.580557	3.579472	-0.386637
C	-2.723216	5.200684	1.026512	H	-5.343622	2.400020	0.158828
C	-1.194763	1.032034	3.181162	H	-0.693827	3.579098	-0.703003
O	-1.515388	0.844376	4.359372	C	-0.354379	5.824515	1.429244
O	-0.724396	-0.037922	2.427050	C	0.939384	5.344604	1.729820
C	-3.699099	4.233920	0.679819	C	-0.611551	7.203391	1.608361
H	-3.334331	3.259072	0.343517	C	1.924662	6.199768	2.221548
H	-3.044826	6.150194	1.454295	H	1.147486	4.283990	1.582286
C	-0.657454	-1.283794	3.093106	C	0.382533	8.061468	2.076244
H	0.010640	-1.247361	3.970833	H	-1.587364	7.619934	1.352516
H	-1.648624	-1.617574	3.446253	C	1.652430	7.562469	2.392649
H	-0.265841	-2.009941	2.365966	H	2.913424	5.803967	2.465911
N	-5.001062	4.394218	0.745079	H	0.168209	9.126722	2.191628
C	-5.609389	5.658062	1.172669	H	2.429119	8.235990	2.763491



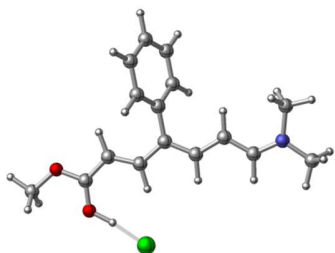
Zero-point correction= 0.314328 (Hartree/Particle)
 Thermal correction to Energy= 0.333698
 Thermal correction to Enthalpy= 0.334642
 Thermal correction to Gibbs Free Energy= 0.263809
 Sum of electronic and zero-point Energies= -825.392440
 Sum of electronic and thermal Energies= -825.373071
 Sum of electronic and thermal Enthalpies= -825.372127
 Sum of electronic and thermal Free Energies= -825.442959

3a-OH

E(scf) = -1286.45284976 a.u.

$\nu_{\min} = 15.90 \text{ cm}^{-1}$

C	-0.143938	2.242736	0.406707	C	3.308691	4.522460	1.639671
C	-1.494442	2.600841	0.391816	H	2.864487	5.199459	0.891874
C	-2.419022	1.612506	-0.032599	H	2.705834	4.579600	2.560993
H	0.082032	1.223241	0.069500	H	4.325636	4.865954	1.863554
H	-1.982564	0.642556	-0.294295	C	4.662873	2.511692	1.056053
C	-3.789079	1.744556	-0.161554	H	5.334775	3.079902	0.391981
H	-4.299142	2.679460	0.073453	H	5.128172	2.454870	2.053969
C	0.948858	3.030563	0.816861	H	4.555680	1.493709	0.660020
C	-4.633313	0.693766	-0.606576	C	-1.948072	3.963638	0.800193
O	-4.320899	-0.498049	-0.947952	C	-2.809328	4.136486	1.899095
O	-5.919929	1.004922	-0.670555	C	-1.527465	5.105641	0.094478
C	2.240162	2.520977	0.772515	C	-3.235868	5.411647	2.281867
H	2.387969	1.499326	0.407209	H	-3.142959	3.259384	2.459098
H	0.767689	4.045059	1.174556	C	-1.951590	6.381761	0.476986
C	-6.852395	0.008700	-1.113137	H	-0.863380	4.986772	-0.765306
H	-6.614468	-0.318146	-2.135929	C	-2.807972	6.539141	1.572246
H	-6.834842	-0.863680	-0.443728	H	-3.902977	5.525226	3.140402
H	-7.836165	0.491089	-1.085679	H	-1.615300	7.256497	-0.085894
N	3.358835	3.155816	1.135666	H	-3.141094	7.536291	1.871194



Zero-point correction=	0.326410 (Hartree/Particle)
Thermal correction to Energy=	0.348189
Thermal correction to Enthalpy=	0.349133
Thermal correction to Gibbs Free Energy=	0.271823
Sum of electronic and zero-point Energies=	-1286.126440
Sum of electronic and thermal Energies=	-1286.104661
Sum of electronic and thermal Enthalpies=	-1286.103717
Sum of electronic and thermal Free Energies=	-1286.181027

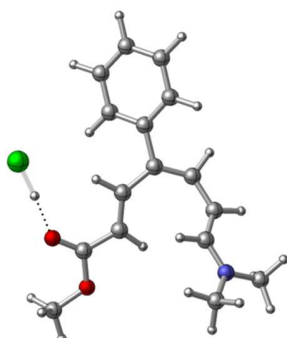
3a-OH-aii

E(scf) = -1286.43850809 a.u.

$\nu_{\min} = 14.97 \text{ cm}^{-1}$

C	-0.161400	4.153602	0.523372	N	2.110959	1.762012	2.310653
C	-1.530733	3.972769	0.703432	C	3.380857	1.881090	1.611805
C	-2.210624	2.730197	1.014316	H	4.081324	1.128480	1.994585
H	0.099994	5.085922	0.007947	H	3.245486	1.717188	0.530736
H	-3.256799	2.847744	1.312820	H	3.825654	2.881394	1.756035
C	-1.787720	1.437116	0.902868	C	2.071780	0.929523	3.503640
H	-0.776913	1.172483	0.594579	H	2.374150	-0.103328	3.265018
C	0.989281	3.392289	0.889719	H	2.754081	1.318329	4.279297
C	-2.673068	0.320000	1.181034	H	1.053360	0.909637	3.913019
O	-3.863847	0.366575	1.507624	C	-2.413780	5.154085	0.467627
O	-2.047485	-0.861930	1.057174	C	-3.689565	5.016357	-0.121268
C	1.041359	2.475050	1.921088	C	-1.999713	6.456504	0.822743
H	0.142999	2.299454	2.517249	C	-4.506384	6.126368	-0.348489
H	1.917362	3.664795	0.381612	H	-4.054125	4.029436	-0.411316
C	-2.827300	-2.038365	1.286677	C	-2.810952	7.568633	0.583368
H	-3.215363	-2.056145	2.316534	H	-1.036926	6.596661	1.320133
H	-3.678456	-2.086008	0.590397	C	-4.071238	7.410775	-0.003439
H	-2.153522	-2.887661	1.120954	H	-5.489412	5.984005	-0.805565

H	-2.462302	8.563394	0.874053	H	-4.710592	8.278866	-0.183101
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Zero-point correction=	0.325664 (Hartree/Particle)
Thermal correction to Energy=	0.347798
Thermal correction to Enthalpy=	0.348743
Thermal correction to Gibbs Free Energy=	0.270368
Sum of electronic and zero-point Energies=	-1286.112844
Sum of electronic and thermal Energies=	-1286.090710
Sum of electronic and thermal Enthalpies=	-1286.089765
Sum of electronic and thermal Free Energies=	-1286.168140

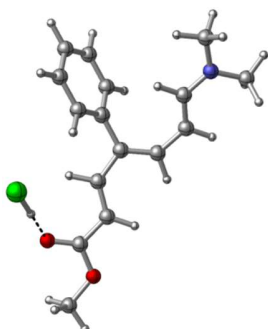
3a-OH-int

E(scf) = -1286.44398626 a.u.

$\nu_{\min} = 15.89 \text{ cm}^{-1}$

C	-0.193651	2.033997	0.572156	H	-4.688564	-1.873835	-3.120105
C	-1.396229	2.577373	0.140360	H	-4.068700	-3.315461	-2.234776
C	-2.407442	1.752232	-0.471608	N	1.845592	4.234701	2.831948
H	-0.026673	0.992182	0.277033	C	3.134917	3.564710	2.903093
H	-3.286009	2.297318	-0.828263	H	3.045066	2.576874	3.387250
C	-2.437336	0.395975	-0.656694	H	3.554472	3.416551	1.894688
H	-1.621714	-0.262043	-0.351782	H	3.833941	4.177108	3.485801
C	0.878193	2.564612	1.348220	C	1.657483	5.428543	3.643026
C	-3.570199	-0.246978	-1.287342	H	1.754493	5.195295	4.717278
O	-4.655050	0.275832	-1.581664	H	2.409257	6.193202	3.387051
O	-3.352676	-1.547000	-1.543455	H	0.658880	5.848324	3.464669
C	0.844605	3.732386	2.091821	C	-1.729477	4.029910	0.264647
H	-0.072699	4.322218	2.119860	C	-2.905176	4.450403	0.911872
H	1.773368	1.941111	1.397647	C	-0.893179	5.011745	-0.302575
C	-4.426944	-2.283885	-2.132703	C	-3.222533	5.810192	1.011218
H	-5.321610	-2.252966	-1.492228	H	-3.583519	3.703326	1.330583

C	-1.207008	6.367828	-0.202249	H	-4.140749	6.114745	1.520510
H	0.018913	4.699143	-0.817031	H	-0.543959	7.112945	-0.650078
C	-2.372646	6.774235	0.461414	H	-2.619232	7.836170	0.540264



Zero-point correction=	0.325593 (Hartree/Particle)
Thermal correction to Energy=	0.347742
Thermal correction to Enthalpy=	0.348686
Thermal correction to Gibbs Free Energy=	0.270400
Sum of electronic and zero-point Energies=	-1286.118393
Sum of electronic and thermal Energies=	-1286.096244
Sum of electronic and thermal Enthalpies=	-1286.095300
Sum of electronic and thermal Free Energies=	-1286.173586

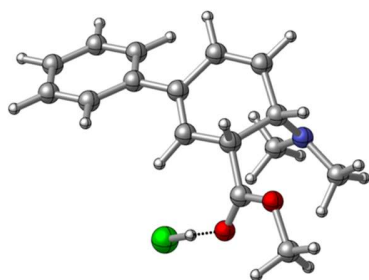
3a-OH-p1

E(scf) = -1286.44788814a.u.

$\nu_{\min} = 31.09 \text{ cm}^{-1}$

C	-1.414723	4.544623	0.920456	H	-5.343047	-1.082934	0.300550
C	-1.123515	3.402600	1.807424	H	-6.511466	0.241537	0.601250
C	-1.914268	2.306102	1.728245	H	-6.132126	-0.248620	-1.091735
H	-1.790733	1.475006	2.422677	N	-4.710370	4.071159	1.239919
C	-2.971750	2.212244	0.670262	C	-4.379939	4.220369	2.646048
H	-2.479655	1.951828	-0.286393	H	-4.286993	3.253637	3.181825
C	-2.572276	4.644312	0.240126	H	-3.429954	4.759348	2.765359
C	-3.994697	1.131904	0.917300	H	-5.166766	4.807108	3.147799
O	-4.227048	0.585639	1.984141	C	-6.048124	3.550423	1.018641
O	-4.671008	0.836803	-0.188754	H	-6.225907	2.558031	1.485446
C	-3.663750	3.599577	0.352603	H	-6.793280	4.240705	1.448919
H	-4.130430	3.476135	-0.635314	H	-6.251810	3.459978	-0.058601
H	-2.802198	5.534915	-0.350772	H	-0.673732	5.345256	0.849557
C	-5.729804	-0.126790	-0.079805	C	-0.025746	3.508629	2.801910

C	0.714512	2.375194	3.194350	H	-0.272280	5.639767	3.126233
C	0.291989	4.744924	3.398790	C	2.021654	3.705795	4.744187
C	1.722766	2.471506	4.155354	H	2.286037	1.578663	4.439132
H	0.509338	1.410917	2.724030	H	1.523036	5.810702	4.815654
C	1.301633	4.841813	4.360501	H	2.813705	3.781803	5.493393



Zero-point correction=	0.328495 (Hartree/Particle)
Thermal correction to Energy=	0.348947
Thermal correction to Enthalpy=	0.349891
Thermal correction to Gibbs Free Energy=	0.278219
Sum of electronic and zero-point Energies=	-1286.119393
Sum of electronic and thermal Energies=	-1286.098941
Sum of electronic and thermal Enthalpies=	-1286.097997
Sum of electronic and thermal Free Energies=	-1286.169669

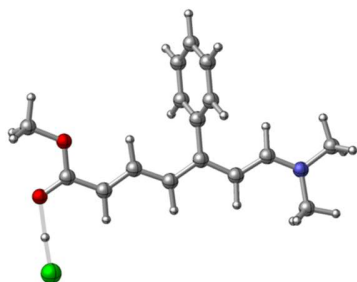
3b-OH

E(scf) = -1286.45285742 a.u.

$\nu_{\min} = 16.79 \text{ cm}^{-1}$

C	-0.043420	1.823157	0.275282	C	-5.451282	-1.337960	-1.492057
C	-1.392970	2.145945	0.285908	H	-6.152053	-1.584759	-0.680049
C	-2.448312	1.296747	-0.143282	H	-6.019204	-0.896051	-2.324863
H	-2.183753	0.309058	-0.531538	H	-4.927515	-2.241058	-1.827935
C	-3.778796	1.627508	-0.113270	N	3.247730	3.392059	1.143625
H	-4.113071	2.595438	0.266118	C	2.924441	4.779561	1.433385
C	0.937890	2.792727	0.662935	H	2.423466	5.254910	0.573437
C	-4.835782	0.751223	-0.566383	H	2.255086	4.860228	2.307472
O	-6.044101	1.036546	-0.543270	H	3.846531	5.333526	1.648650
O	-4.437149	-0.440168	-1.034205	C	4.631432	2.971638	1.298055
C	2.285199	2.520329	0.790197	H	5.295166	3.562545	0.644713
H	2.643146	1.506190	0.594972	H	4.970418	3.101784	2.340298
H	0.566294	3.793806	0.893182	H	4.733524	1.911806	1.029934

H	-6.450156	2.422086	0.003588	C	1.570553	-1.000012	-1.704923
C				H	1.421548	1.147157	-1.918356
I	-6.762470	3.660422	0.496131	C	0.488583	-1.947377	0.240626
H	-1.669802	3.147488	0.634256	H	-0.513339	-0.540175	1.543509
C	0.402426	0.457016	-0.140708	C	1.237102	-2.115917	-0.929040
C	1.160472	0.276928	-1.311394	H	2.151559	-1.123941	-2.622389
C	0.072366	-0.670801	0.630536				



Zero-point correction= 0.325404 (Hartree/Particle)

Thermal correction to Energy= 0.347567

Thermal correction to Enthalpy= 0.348511

Thermal correction to Gibbs Free Energy= 0.269734

Sum of electronic and zero-point Energies= -1286.127453

Sum of electronic and thermal Energies= -1286.105290

Sum of electronic and thermal Enthalpies= -1286.104346

Sum of electronic and thermal Free Energies= -1286.183123

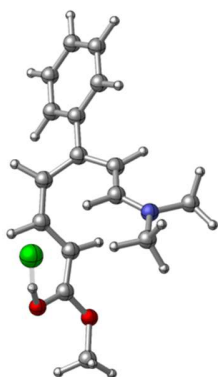
3b-OH-aii

E(scf) = -1286.44319050 a.u.

$\nu_{\min} = 29.09 \text{ cm}^{-1}$

C	-0.827698	4.921687	1.445837	H	-3.705901	-0.943243	3.828275
C	-0.173604	3.672910	1.294216	H	-2.175518	-1.477541	4.590507
C	-0.566874	2.421346	1.793076	H	-3.416570	-0.628371	5.579223
H	-0.077190	1.560543	1.326249	N	-4.392072	3.935510	1.499688
C	-1.411243	2.128594	2.873408	C	-5.058396	4.933455	2.328932
H	-1.787845	2.916929	3.526634	H	-4.482745	5.111233	3.249527
C	-2.228524	5.038975	1.621708	H	-5.161711	5.889615	1.788954
C	-1.821334	0.825508	3.154186	H	-6.058356	4.573249	2.599440
O	-1.725516	-0.184614	2.341113	C	-5.216141	2.884633	0.905089
O	-2.375522	0.591972	4.339519	H	-5.801740	2.385232	1.692356
C	-3.096946	4.019426	1.222969	H	-5.917683	3.315105	0.170869
H	-2.706427	3.190125	0.622161	H	-4.570399	2.143285	0.413315
H	-2.630581	5.970978	2.022271	H	0.755556	3.679506	0.716144
C	-2.950412	-0.696715	4.589158	C	-0.015729	6.162006	1.362012

C	1.318901	6.177540	1.817125	H	-1.575533	7.355804	0.444803
C	-0.553487	7.352144	0.829556	C	1.538020	8.513740	1.213870
C	2.086774	7.341075	1.745593	H	3.116172	7.335081	2.112408
H	1.745954	5.271983	2.253450	H	-0.215913	9.423815	0.328974
C	0.215531	8.514547	0.754896	H	2.139479	9.424457	1.156421



Zero-point correction= 0.328361 (Hartree/Particle)

Thermal correction to Energy= 0.349587

Thermal correction to Enthalpy= 0.350532

Thermal correction to Gibbs Free Energy= 0.276487

Sum of electronic and zero-point Energies= -1286.114830

Sum of electronic and thermal Energies= -1286.093603

Sum of electronic and thermal Enthalpies= -1286.092659

Sum of electronic and thermal Free Energies= -1286.166703

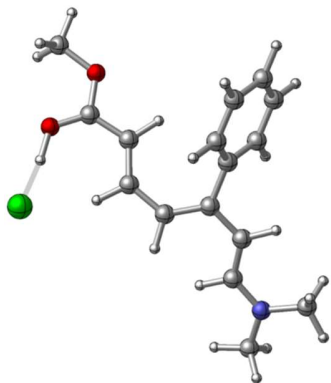
3b-OH-int

E(scf) = -1286.43931515 a.u.

$\nu_{\min} = 12.76 \text{ cm}^{-1}$

C	-2.216660	4.271121	1.244500	H	-2.965816	6.113473	0.426335
C	-2.251703	2.872135	1.300643	C	1.276414	0.668334	5.845691
C	-1.532383	1.977136	2.131183	H	0.561701	-0.043376	6.284511
H	-1.700352	0.922282	1.889194	H	2.021455	0.111181	5.258901
C	-0.700574	2.224301	3.209929	H	1.768684	1.248524	6.634807
H	-0.499247	3.231204	3.570762	N	-5.373818	5.268295	-0.498530
C	-3.204959	5.060330	0.580519	C	-5.135754	6.642152	-0.920057
C	-0.076747	1.194479	3.964399	H	-5.077405	7.320272	-0.051504
O	-0.085495	-0.064408	3.768485	H	-4.191780	6.715659	-1.482236
O	0.597816	1.627133	5.024443	H	-5.957023	6.972080	-1.567883
C	-4.442508	4.583097	0.174627	C	-6.695868	4.709287	-0.747352
H	-4.729129	3.558032	0.425785	H	-7.469487	5.284433	-0.211086

H	-6.927667	4.736945	-1.824187	H	0.432463	3.968983	0.741604
H	-6.733907	3.667285	-0.404688	C	-0.267730	6.805769	3.306383
H	-2.962137	2.376628	0.633700	H	-2.356784	6.300398	3.056820
C	-1.086813	5.042974	1.839800	C	1.047541	6.522643	2.924213
C	0.239419	4.770424	1.458072	H	2.321981	5.288107	1.682213
C	-1.329233	6.078615	2.758584	H	-0.469767	7.597169	4.032578
C	1.297127	5.507306	1.992154	H	1.877166	7.094010	3.348129



Zero-point correction=	0.325259 (Hartree/Particle)
Thermal correction to Energy=	0.347171
Thermal correction to Enthalpy=	0.348115
Thermal correction to Gibbs Free Energy=	0.270258
Sum of electronic and zero-point Energies=	-1286.114056
Sum of electronic and thermal Energies=	-1286.092144
Sum of electronic and thermal Enthalpies=	-1286.091200
Sum of electronic and thermal Free Energies=	-1286.169057

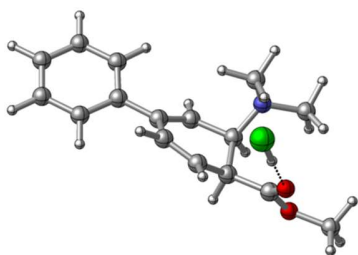
3b-OH-p1

E(scf) = -1286.44664323 a.u.

$\nu_{\min} = 30.13 \text{ cm}^{-1}$

C	-1.659998	4.335996	0.261976	O	-4.982844	0.521511	0.873653
C	-1.053188	3.063834	-0.172852	C	-3.925813	3.228877	0.173240
C	-1.747422	1.912521	-0.165593	H	-4.724235	3.240232	0.929042
H	-1.314820	0.990482	-0.556799	H	-3.488844	5.339251	0.711391
C	-3.126963	1.888007	0.424779	C	-5.892436	-0.553209	0.592427
H	-3.022233	1.855467	1.525773	H	-6.366615	-0.403993	-0.389110
C	-3.002168	4.398528	0.443195	H	-5.362762	-1.516503	0.593071
C	-3.947258	0.678540	0.054565	H	-6.645637	-0.526767	1.387856
O	-3.742275	-0.077431	-0.881857	N	-4.584315	3.411558	-1.108101

C	-3.761386	3.336267	-2.301698	C	-1.221687	6.818749	0.105894
H	-3.444268	2.303632	-2.553971	C	0.519170	5.379365	0.962528
H	-4.324757	3.733121	-3.162098	C	-0.396864	7.929681	0.295690
H	-2.853495	3.943755	-2.183509	H	-2.213820	6.952851	-0.331130
C	-5.892647	2.803385	-1.273593	C	1.344539	6.490871	1.154636
H	-5.855880	1.729191	-1.555149	H	0.884290	4.387032	1.238156
H	-6.476719	2.890452	-0.345465	C	0.890202	7.771446	0.822724
H	-6.446832	3.321614	-2.074422	H	-0.757305	8.924201	0.020054
H	-0.030174	3.083682	-0.556064	H	2.347314	6.354995	1.567999
C	-0.781994	5.523546	0.442864	H	1.536846	8.640514	0.967764



Zero-point correction=	0.328410 (Hartree/Particle)
Thermal correction to Energy=	0.348892
Thermal correction to Enthalpy=	0.349836
Thermal correction to Gibbs Free Energy=	0.278044
Sum of electronic and zero-point Energies=	-1286.118234
Sum of electronic and thermal Energies=	-1286.097751
Sum of electronic and thermal Enthalpies=	-1286.096807
Sum of electronic and thermal Free Energies=	-1286.168599

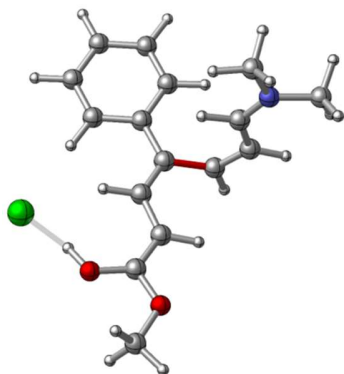
TS-3a-OH-r

E(scf) = -1286.41596930 a.u.

$\nu_{\min} = -127.07 \text{ cm}^{-1}$

C	-0.347149	3.054713	-0.412744	H	-3.599301	-2.807476	1.201933
C	-1.715600	3.236899	0.133040	H	-4.055910	-2.648894	-0.520079
C	-2.488720	2.118916	0.332977	H	-2.562222	-3.544985	-0.069204
H	-0.236763	2.977835	-1.503954	N	1.689090	2.988959	2.609753
H	-3.498130	2.270040	0.726463	C	3.107823	2.909681	2.251161
C	-2.100834	0.768936	0.093997	H	3.504462	1.934848	2.571836
H	-1.094431	0.528688	-0.254239	H	3.256534	3.031440	1.175106
C	0.792874	2.957164	0.322844	H	3.648810	3.704884	2.783130
C	-2.925799	-0.325220	0.283679	C	1.425602	3.021375	4.052862
O	-4.177191	-0.360228	0.662092	H	1.865330	2.127273	4.518637
O	-2.381143	-1.534461	0.067388	H	1.895726	3.916077	4.486681
C	0.708558	3.015949	1.751322	H	0.346098	3.041783	4.240171
H	-0.298944	3.083357	2.175477	C	-2.187099	4.616724	0.377408
H	1.753743	2.825318	-0.175595	C	-3.560994	4.904097	0.581476
C	-3.206872	-2.692503	0.179697	C	-1.288168	5.709052	0.407321

C	-3.992657	6.205564	0.830606	C	-3.084981	7.274073	0.869823
H	-4.304176	4.103597	0.536186	H	-5.059283	6.390037	0.987739
C	-1.730372	7.013445	0.650282	H	-1.003838	7.830727	0.667701
H	-0.221696	5.543202	0.243834	H	-3.432510	8.292487	1.060598



Zero-point correction=	0.327698 (Hartree/Particle)
Thermal correction to Energy=	0.348937
Thermal correction to Enthalpy=	0.349881
Thermal correction to Gibbs Free Energy=	0.274255
Sum of electronic and zero-point Energies=	-1286.088272
Sum of electronic and thermal Energies=	-1286.067032
Sum of electronic and thermal Enthalpies=	-1286.066088
Sum of electronic and thermal Free Energies=	-1286.141714

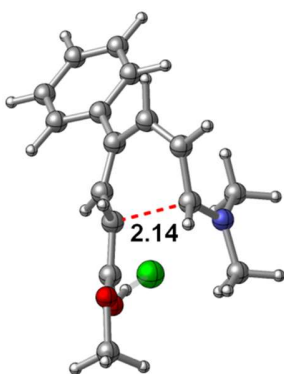
TS-3a-OH-uu

E(scf) = -1286.42107884 a.u.

$\nu_{\min} = -278.11 \text{ cm}^{-1}$

C	-1.407851	4.304596	0.825019	H	-6.400790	0.075452	0.155430
C	-1.140352	3.216241	1.777606	H	-5.842509	-0.455813	-1.474377
C	-1.932800	2.104397	1.763304	N	-4.650645	4.102066	1.564220
H	-1.883995	1.395179	2.592888	C	-4.178782	4.761263	2.780991
C	-2.888188	1.874351	0.692405	H	-4.072169	4.009838	3.580130
H	-2.528546	2.036049	-0.327875	H	-3.216251	5.250774	2.602532
C	-2.616883	4.568881	0.285579	H	-4.917588	5.518517	3.086034
C	-3.912615	0.905018	0.755093	C	-5.968886	3.488028	1.689749
O	-4.441069	0.552660	-0.411802	H	-5.940975	2.733852	2.493210
C	-3.857052	3.779872	0.539210	H	-6.716019	4.254610	1.947638
H	-4.388034	3.416363	-0.344745	H	-6.258730	3.011535	0.744393
H	-2.760153	5.458929	-0.336868	H	-0.589231	4.993676	0.597246
C	-5.562538	-0.342972	-0.420758	C	-0.080862	3.407652	2.795434
H	-5.283357	-1.316985	0.006274	C	0.611718	2.307769	3.344856

C	0.255506	4.695317	3.263927	C	1.900816	3.770984	4.787996
C	1.583176	2.486259	4.331424	H	2.105891	1.616225	4.737618
H	0.398953	1.301674	2.976611	H	1.467717	5.882989	4.596522
C	1.232759	4.874284	4.246580	H	2.666090	3.910668	5.555591
H	-0.270878	5.569430	2.873179	O	-4.424569	0.367114	1.801174



Zero-point correction=	0.327169 (Hartree/Particle)
Thermal correction to Energy=	0.347299
Thermal correction to Enthalpy=	0.348243
Thermal correction to Gibbs Free Energy=	0.277666
Sum of electronic and zero-point Energies=	-1286.093910
Sum of electronic and thermal Energies=	-1286.073780
Sum of electronic and thermal Enthalpies=	-1286.072836
Sum of electronic and thermal Free Energies=	-1286.143413

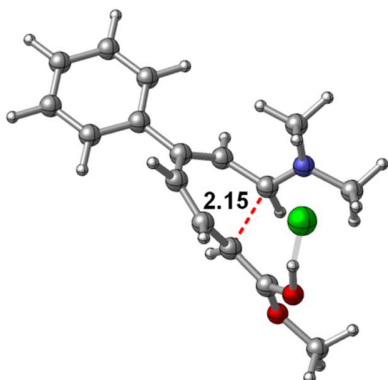
TS-3b-OH-dd

E(scf) = -1286.41917396 a.u.

$\nu_{\min} = -282.80 \text{ cm}^{-1}$

C	-1.752619	4.273347	0.078809	C	-5.738720	-0.566431	1.391029
C	-1.152643	3.008123	-0.370749	H	-6.367915	-0.450739	0.496156
C	-1.782687	1.815148	-0.258512	H	-5.267908	-1.560001	1.372986
H	-1.374370	0.936069	-0.763593	H	-6.342144	-0.448706	2.298470
C	-3.018957	1.694485	0.507376	N	-4.535126	3.289232	-1.482198
H	-3.026503	2.174554	1.490233	C	-3.743862	3.693159	-2.642683
C	-3.102683	4.425459	0.146097	H	-3.303579	2.797314	-3.109405
C	-3.885292	0.586650	0.442235	H	-4.404851	4.194932	-3.366549
O	-3.984057	-0.285634	-0.496527	H	-2.950582	4.384792	-2.341473
O	-4.743328	0.464926	1.451182	C	-5.678804	2.440505	-1.801578
C	-4.112356	3.394147	-0.219620	H	-5.320986	1.527755	-2.305319
H	-4.883722	3.190940	0.528032	H	-6.218507	2.169712	-0.884898
H	-3.537962	5.385052	0.442722	H	-6.365184	2.974830	-2.476829

H	-0.183480	3.066683	-0.872476	C	1.266511	6.219631	1.314167
C	-0.842211	5.409560	0.389993	H	0.697273	4.139827	1.230679
C	-1.191568	6.741792	0.095451	C	0.901498	7.538605	1.024743
C	0.406181	5.166028	0.994198	H	-0.617560	8.820532	0.166527
C	-0.330171	7.794693	0.410962	H	2.226428	6.008614	1.792337
H	-2.137538	6.953814	-0.407984	H	1.576274	8.362875	1.269020



Zero-point correction=	0.327239 (Hartree/Particle)
Thermal correction to Energy=	0.347407
Thermal correction to Enthalpy=	0.348352
Thermal correction to Gibbs Free Energy=	0.277637
Sum of electronic and zero-point Energies=	-1286.091935
Sum of electronic and thermal Energies=	-1286.071767
Sum of electronic and thermal Enthalpies=	-1286.070822
Sum of electronic and thermal Free Energies=	-1286.141537

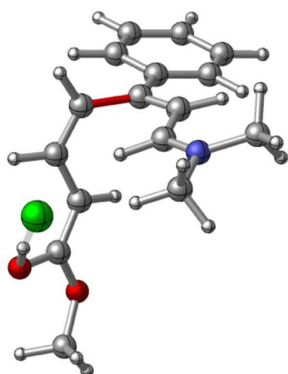
TS-3b-OH-r

E(scf) = -1286.42747508 a.u.

$\nu_{\min} = -44.10\text{cm}^{-1}$

C	-1.240707	4.832446	1.005103	H	-3.124387	2.966760	0.568642
C	-0.717817	3.534045	0.506742	H	-3.005069	6.026253	1.254998
C	-0.590299	2.435978	1.290215	C	-1.585836	0.048852	5.384748
H	-0.370594	1.491362	0.784523	H	-2.617558	-0.164380	5.062351
C	-0.801511	2.374530	2.712043	H	-0.970628	-0.846951	5.208565
H	-0.779967	3.284079	3.315849	H	-1.575398	0.298950	6.453497
C	-2.603376	5.047881	0.991208	N	-4.815472	4.111351	0.653879
C	-1.055821	1.196777	3.365152	C	-5.490120	5.404500	0.802662
O	-1.303154	0.030362	2.794341	H	-5.444540	5.741334	1.849831
O	-1.054018	1.188093	4.710595	H	-5.020346	6.159841	0.158418
C	-3.510954	3.985773	0.712439	H	-6.540459	5.293752	0.510401

C	-5.675282	2.936178	0.479976	C	2.011267	6.629073	1.704012
H	-6.395623	2.893916	1.311544	H	1.424795	4.800283	0.715944
H	-6.234403	3.028471	-0.464011	C	0.209498	7.938076	2.657360
H	-5.061878	2.023749	0.473178	H	-1.770377	7.146975	2.444329
H	-0.594891	3.444663	-0.577158	C	1.576621	7.759840	2.402981
C	-0.295990	5.851636	1.494933	H	3.075502	6.481894	1.505728
C	1.086461	5.684325	1.258938	H	-0.133648	8.812338	3.215535
C	-0.715224	6.997928	2.210602	H	2.299749	8.499338	2.755748



Zero-point correction= 0.328407 (Hartree/Particle)
 Thermal correction to Energy= 0.349179
 Thermal correction to Enthalpy= 0.350123
 Thermal correction to Gibbs Free Energy= 0.277134
 Sum of electronic and zero-point Energies= -1286.099068
 Sum of electronic and thermal Energies= -1286.078296
 Sum of electronic and thermal Enthalpies= -1286.077352
 Sum of electronic and thermal Free Energies= -1286.150341

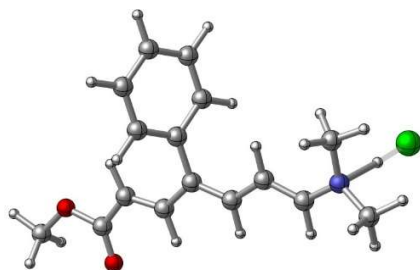
3a-NH

E(scf) = -1286.44749053 a.u.

$\nu_{\min} = 18.3 \text{ cm}^{-1}$

C	-0.188786	2.158861	0.407572	C	2.206852	2.504743	0.731128
C	-1.513973	2.519762	0.424530	H	2.393302	1.490922	0.361894
C	-2.502574	1.542062	0.018421	H	0.725627	3.968210	1.192989
H	0.044329	1.143383	0.065258	C	-6.954069	0.030274	-0.985906
H	-2.122319	0.548020	-0.244567	H	-6.727951	-0.330724	-2.001502
C	-3.843302	1.723370	-0.084418	H	-6.949626	-0.832898	-0.301936
H	-4.321384	2.676499	0.146765	H	-7.936069	0.519071	-0.969436
C	0.928313	2.966001	0.812530	N	3.363630	3.212690	1.021834
C	-4.714742	0.623710	-0.522329	C	3.228058	4.520825	1.661396
O	-4.361669	-0.505330	-0.812532	H	2.592914	5.174358	1.047210
O	-6.007553	1.015189	-0.571318	H	2.785599	4.436448	2.670060

H	4.219809	4.984602	1.741197	H	-3.085878	3.202254	2.545396
C	4.523046	2.427881	1.460588	C	-1.957657	6.301691	0.490202
H	5.440399	3.010805	1.296253	H	-0.925710	4.889150	-0.781311
H	4.451917	2.162498	2.530229	C	-2.767216	6.472606	1.618173
H	4.589579	1.504037	0.869340	H	-3.802493	5.478352	3.238823
C	-1.951397	3.887742	0.836317	H	-1.640185	7.169543	-0.093711
C	-2.768759	4.072817	1.966108	H	-3.083126	7.473944	1.921678
C	-1.554856	5.020028	0.102606	H	3.934342	3.753789	-0.542463
C	-3.171615	5.353537	2.354900	Cl	4.475642	4.303770	-1.635015



Zero-point correction=	0.326200 (Hartree/Particle)
Thermal correction to Energy=	0.348200
Thermal correction to Enthalpy=	0.349144
Thermal correction to Gibbs Free Energy=	0.271055
Sum of electronic and zero-point Energies=	-1286.121291
Sum of electronic and thermal Energies=	-1286.099291
Sum of electronic and thermal Enthalpies=	-1286.098346
Sum of electronic and thermal Free Energies=	-1286.176436

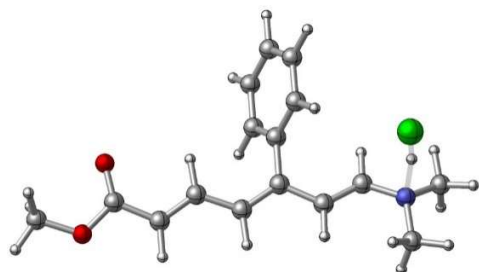
3b-NH

E(scf) = -1286.44790932 a.u.

$\nu_{\min} = 18.5 \text{ cm}^{-1}$

C	0.216220	2.671545	-0.687398	O	-5.506681	1.078548	0.560321
C	-1.146048	2.540807	-0.826426	C	2.300904	3.625867	-1.645401
C	-2.027474	1.856318	0.075288	H	2.826783	3.480528	-0.698724
H	-1.595975	1.350130	0.944496	H	0.445004	3.503502	-2.675319
C	-3.375722	1.774606	-0.074673	C	-6.404718	0.389629	1.429892
H	-3.892979	2.254678	-0.909279	H	-6.163909	-0.684120	1.475104
C	0.984866	3.300620	-1.747630	H	-6.356555	0.798862	2.451275
C	-4.196257	1.032431	0.890816	H	-7.409532	0.533093	1.013499
O	-3.790250	0.439536	1.874679	N	3.128401	4.054815	-2.671965

C	2.528583	4.379632	-3.963213	C	1.961837	1.203047	0.380533
H	1.962833	3.515073	-4.339346	C	1.260489	2.106597	2.931583
H	1.848788	5.247872	-3.893175	H	-0.191315	3.351985	1.923210
H	3.326039	4.608443	-4.682267	C	2.620830	0.702960	1.505980
C	4.287253	4.867762	-2.294235	H	2.248898	0.859128	-0.616186
H	5.043718	4.820199	-3.090365	C	2.272585	1.152665	2.785127
H	4.007953	5.923956	-2.129918	H	0.987653	2.469199	3.925862
H	4.730141	4.472023	-1.369470	H	3.411630	-0.041458	1.382995
H	-1.605663	2.972730	-1.722722	H	2.791575	0.762987	3.664493
C	0.932016	2.154872	0.516777	H	3.776907	2.431261	-2.999884
C	0.594937	2.602677	1.806583	Cl	4.081342	1.153209	-3.238208



Zero-point correction=	0.326183 (Hartree/Particle)
Thermal correction to Energy=	0.348161
Thermal correction to Enthalpy=	0.349105
Thermal correction to Gibbs Free Energy=	0.271647
Sum of electronic and zero-point Energies=	-1286.121727
Sum of electronic and thermal Energies=	-1286.099748
Sum of electronic and thermal Enthalpies=	-1286.098804
Sum of electronic and thermal Free Energies=	-1286.176263

7. Reference

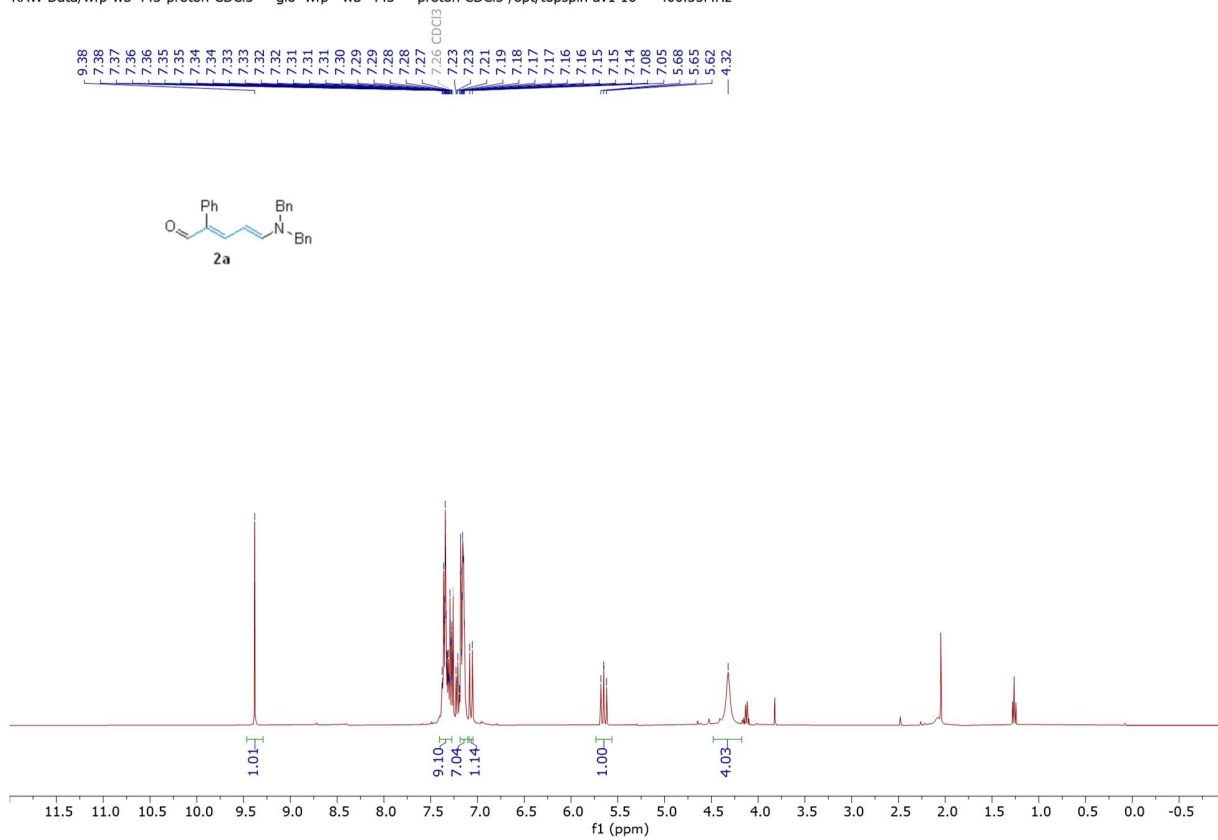
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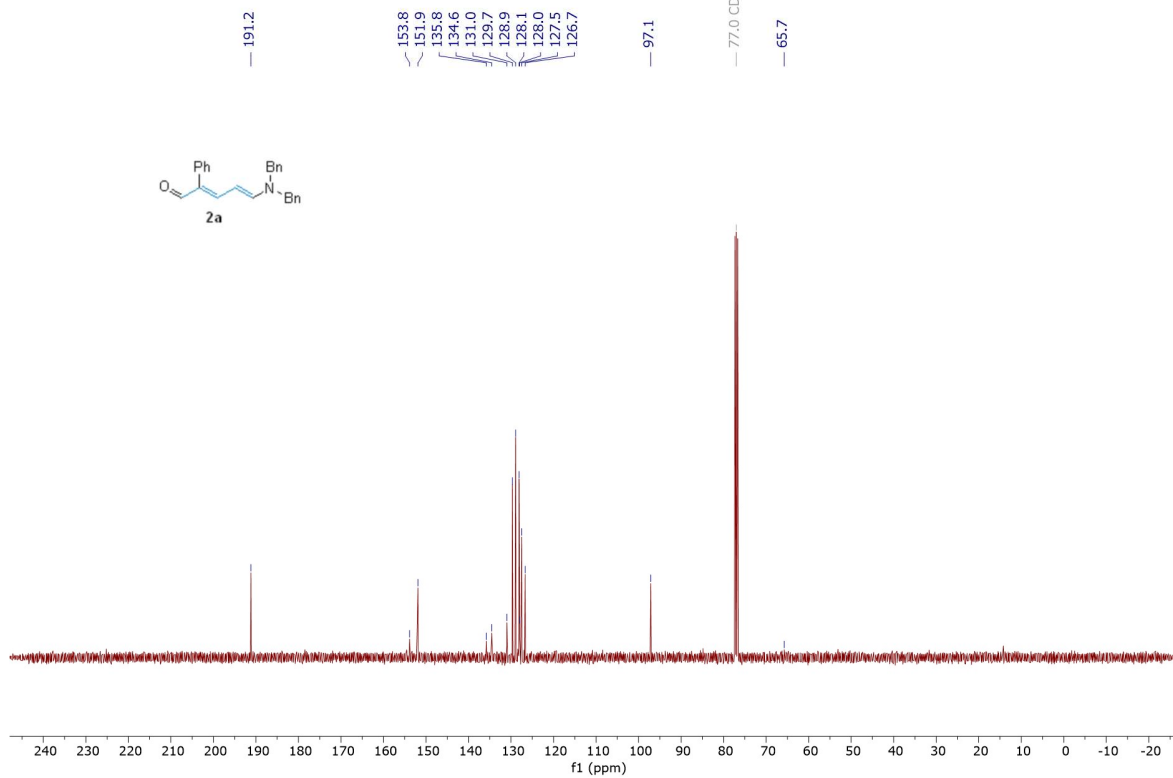
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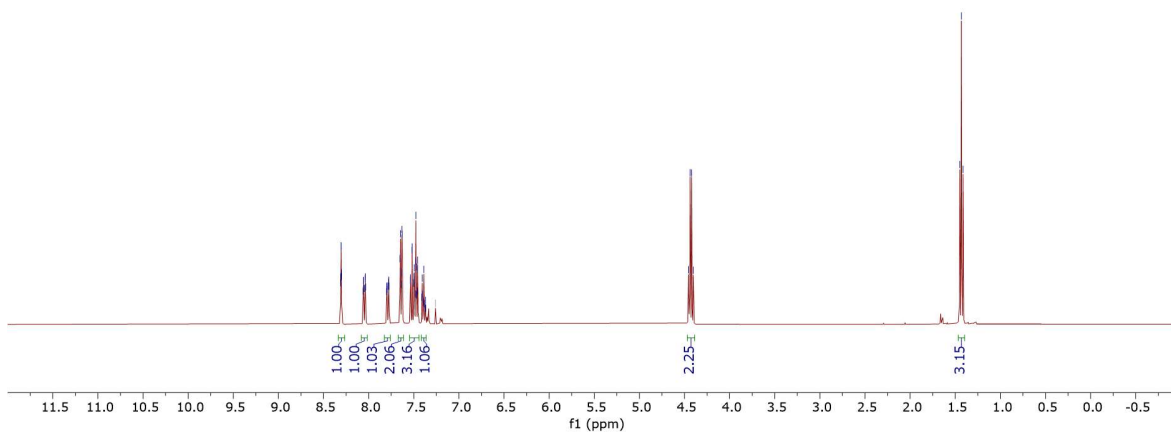
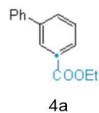


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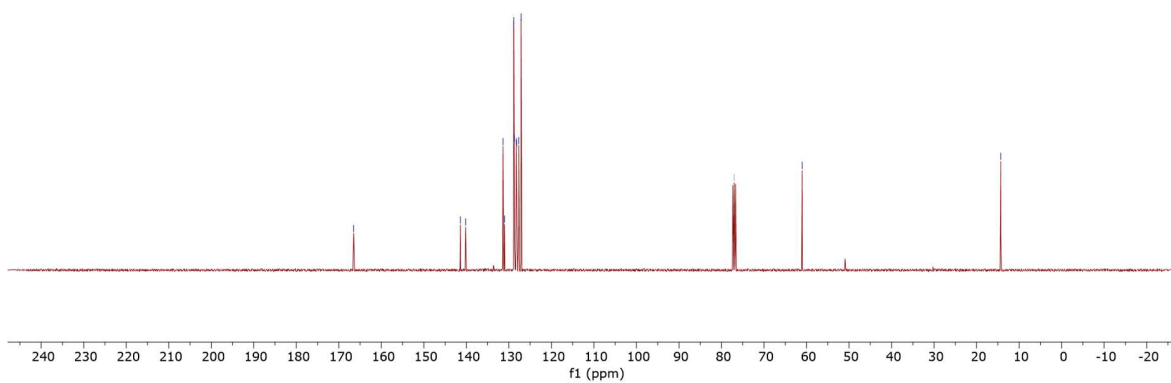
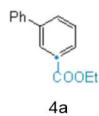
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8.31
8.31
8.31
8.30
8.30
8.30
8.06
8.06
8.06
8.05
8.05
8.04
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8.03
7.80
7.80
7.80
7.79
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7.77
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7.65
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7.64
7.63
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7.52
7.52
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7.49
7.48
7.48
7.47
7.47
7.46
7.46
7.41
7.41
7.40
7.39
7.38
7.37
7.37
7.26 CDCl3
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4.42
4.40
1.45
1.43
1.41

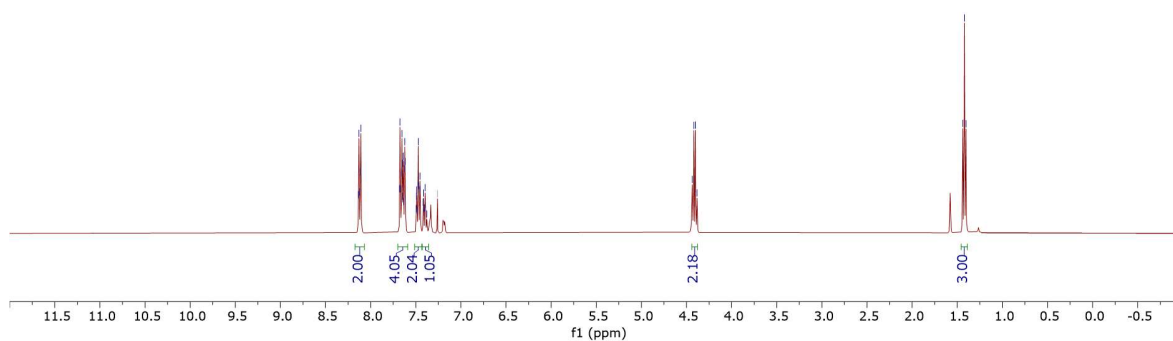
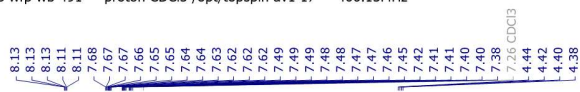


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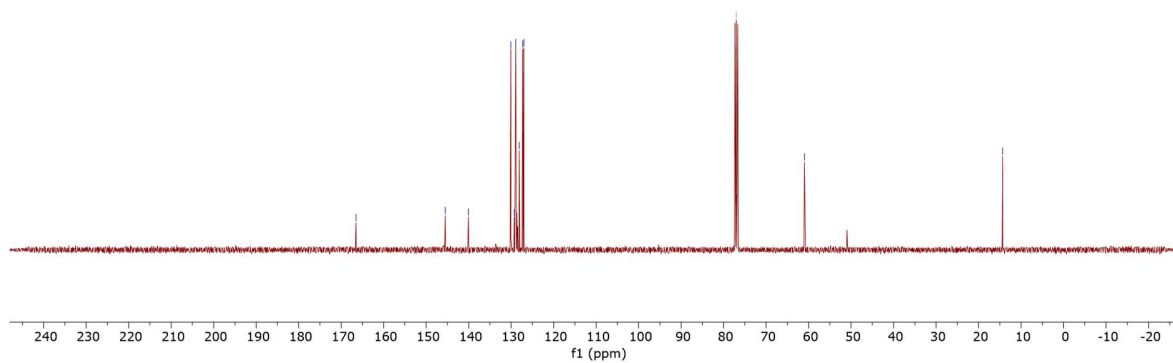
166.5
141.4
140.2
131.4
131.0
128.8
128.8
128.3
128.2
127.7
127.1
77.0 CDCl3
61.0
14.3



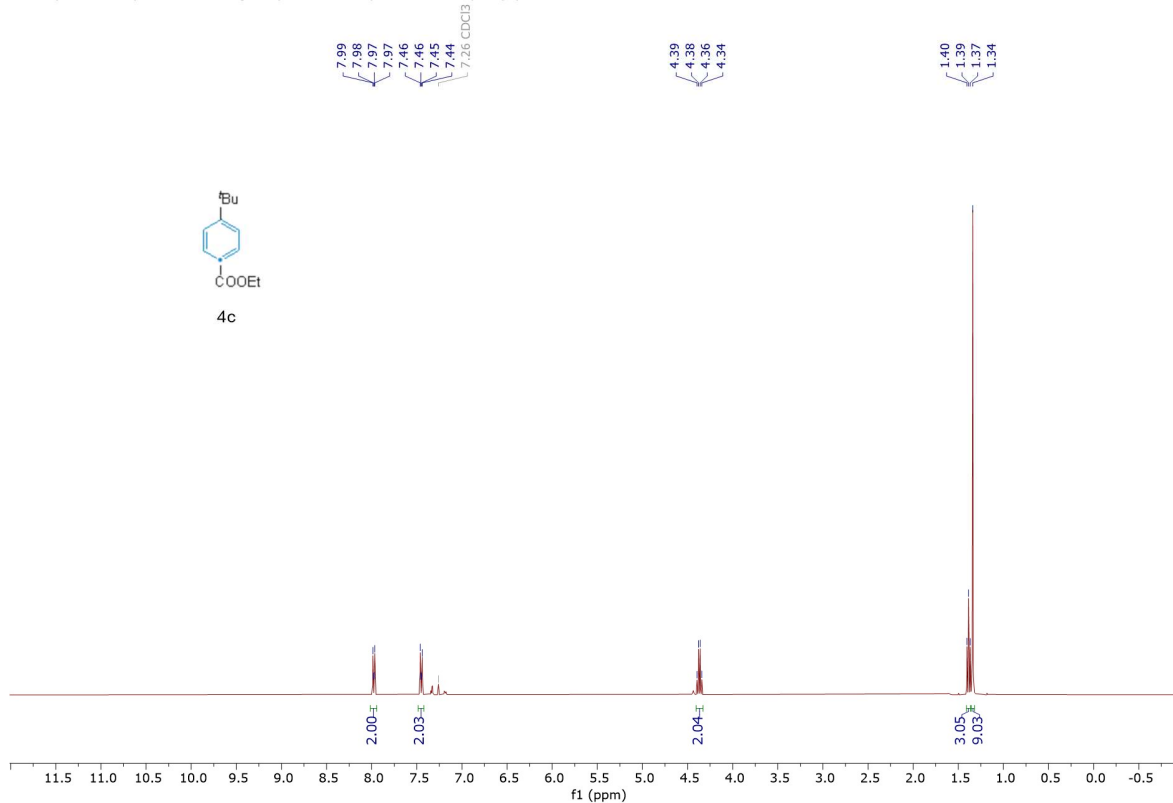
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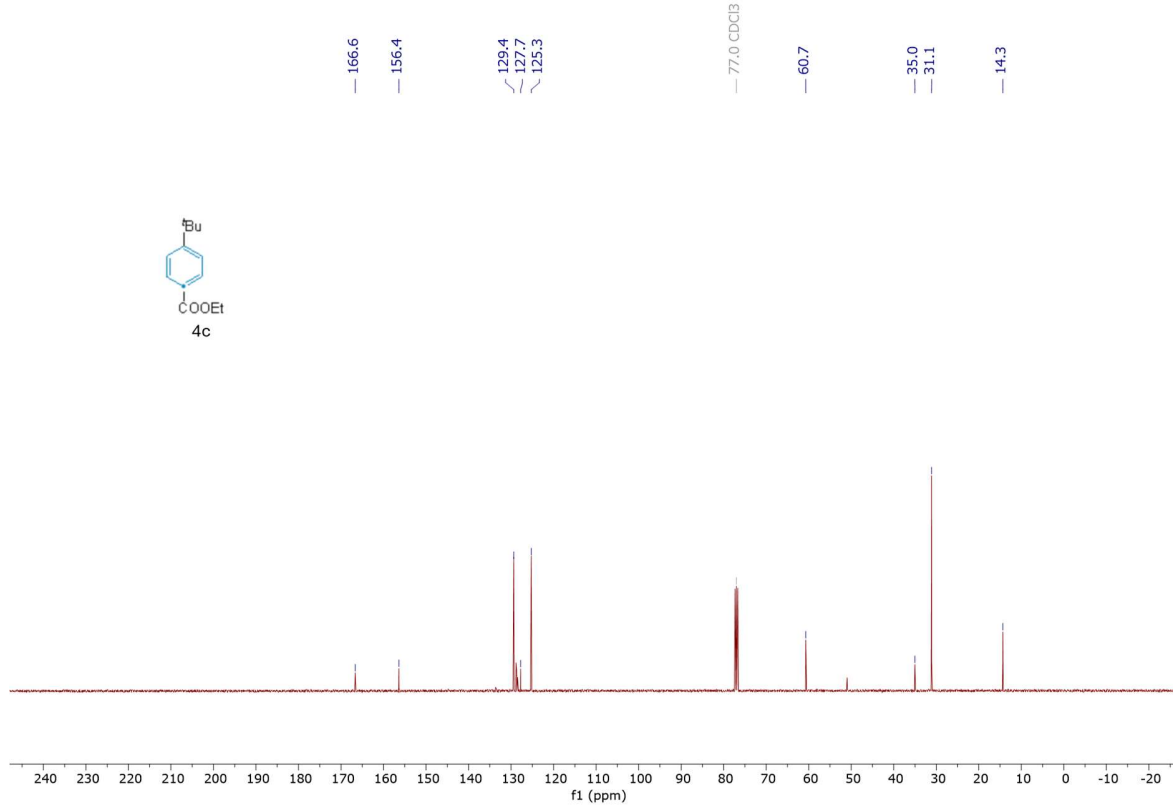
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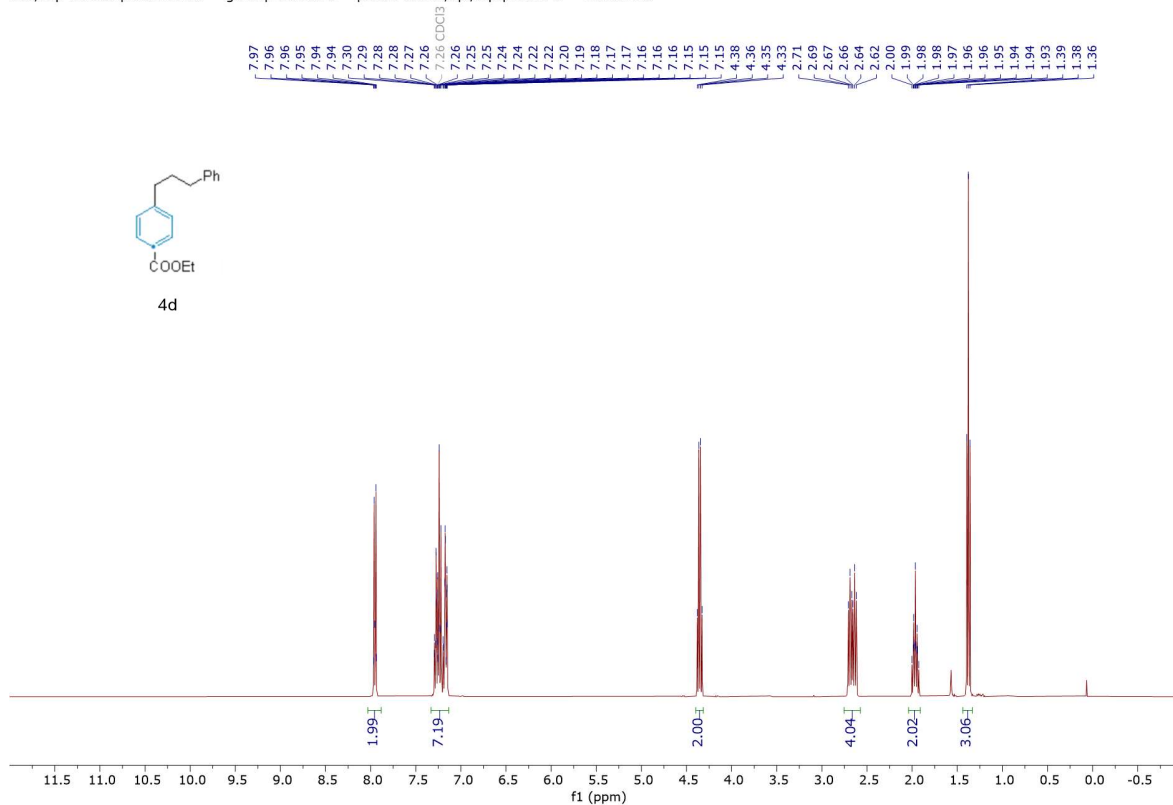
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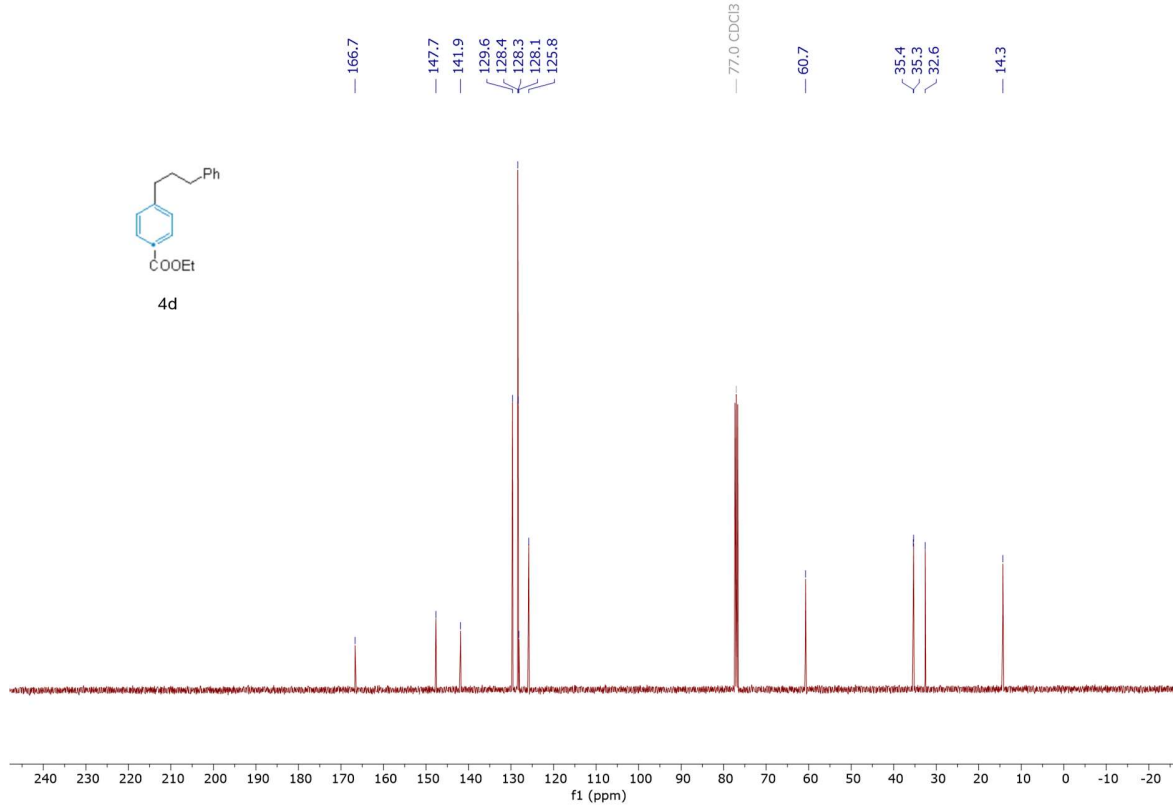
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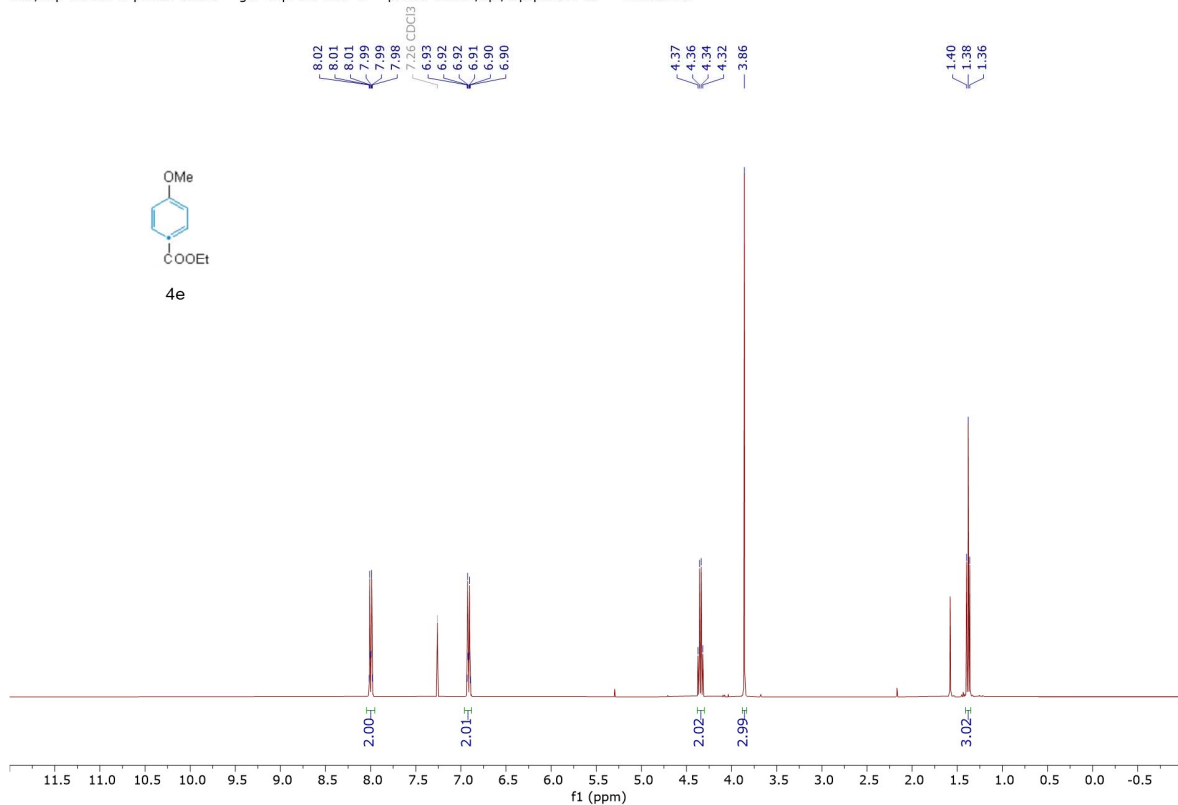
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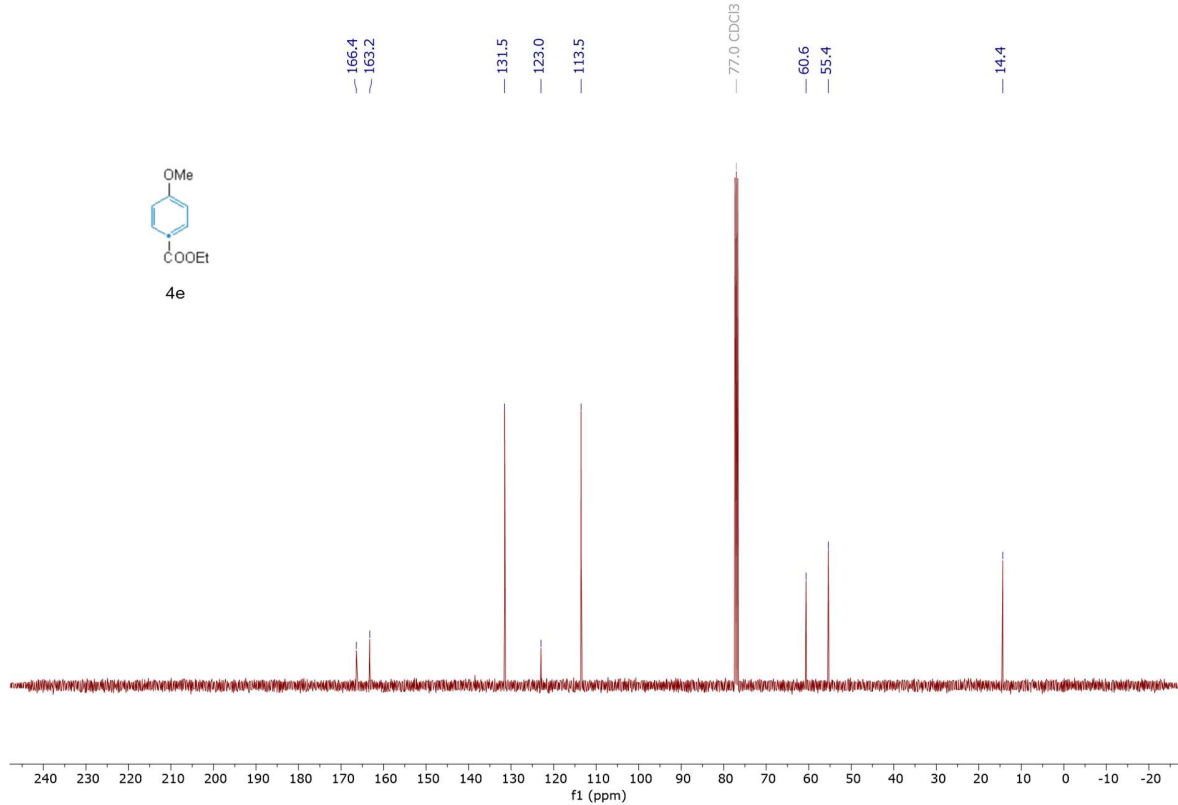
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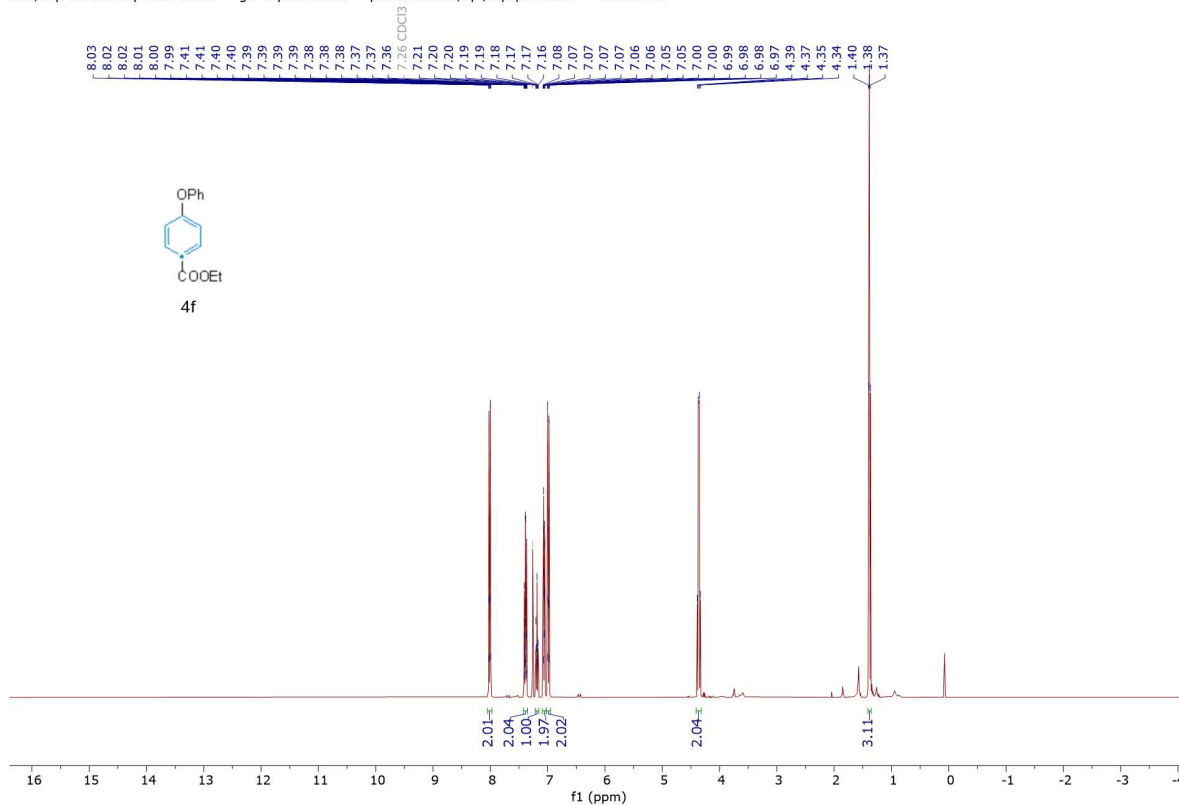
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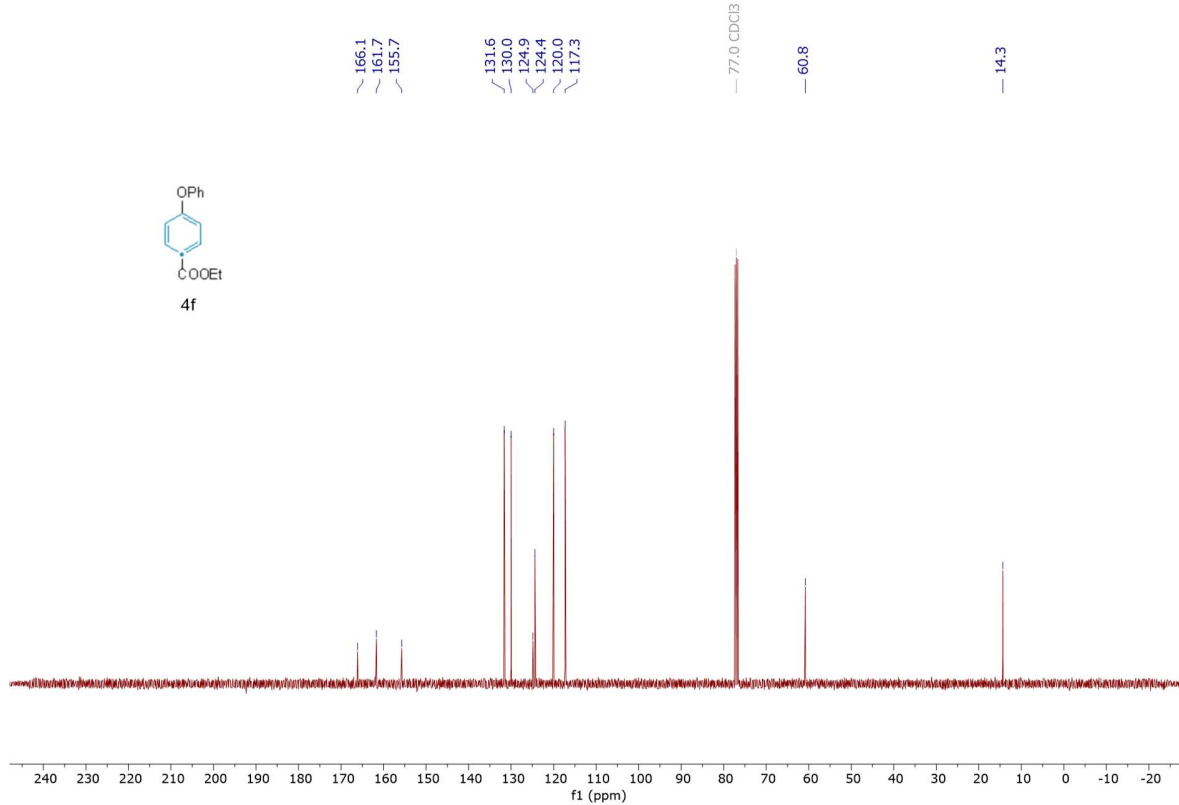
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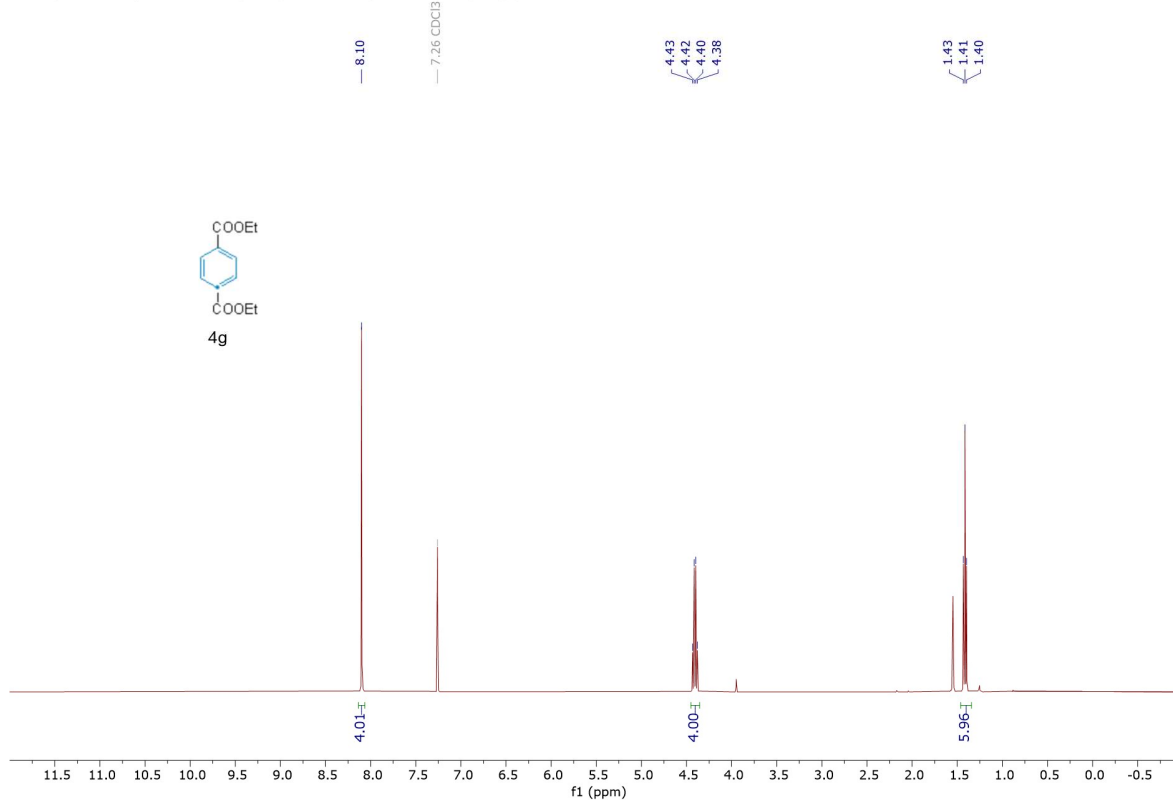
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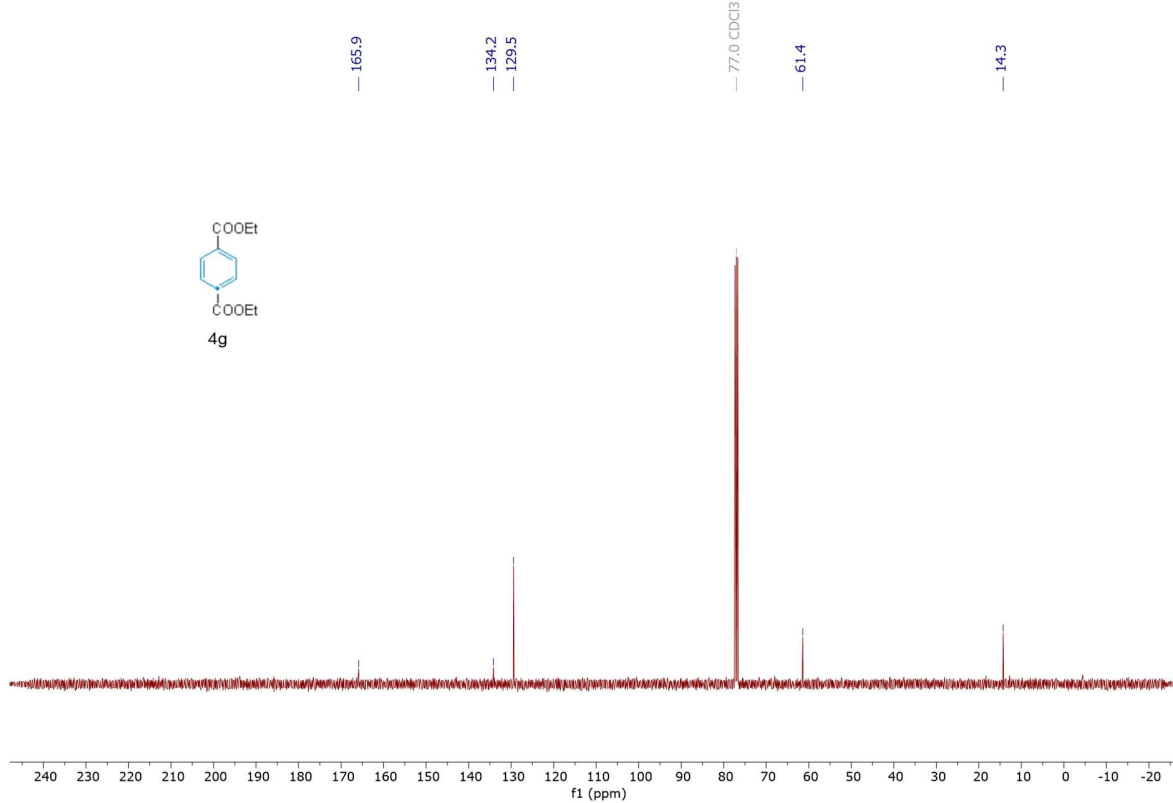
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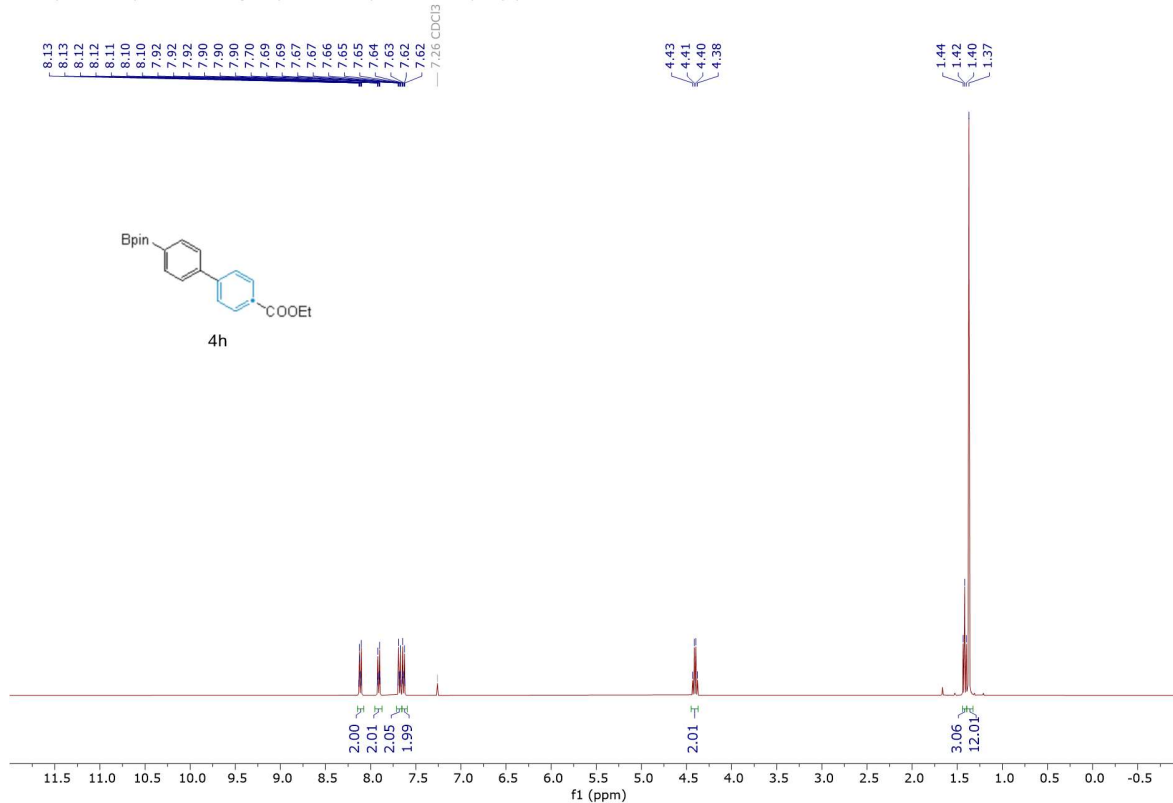
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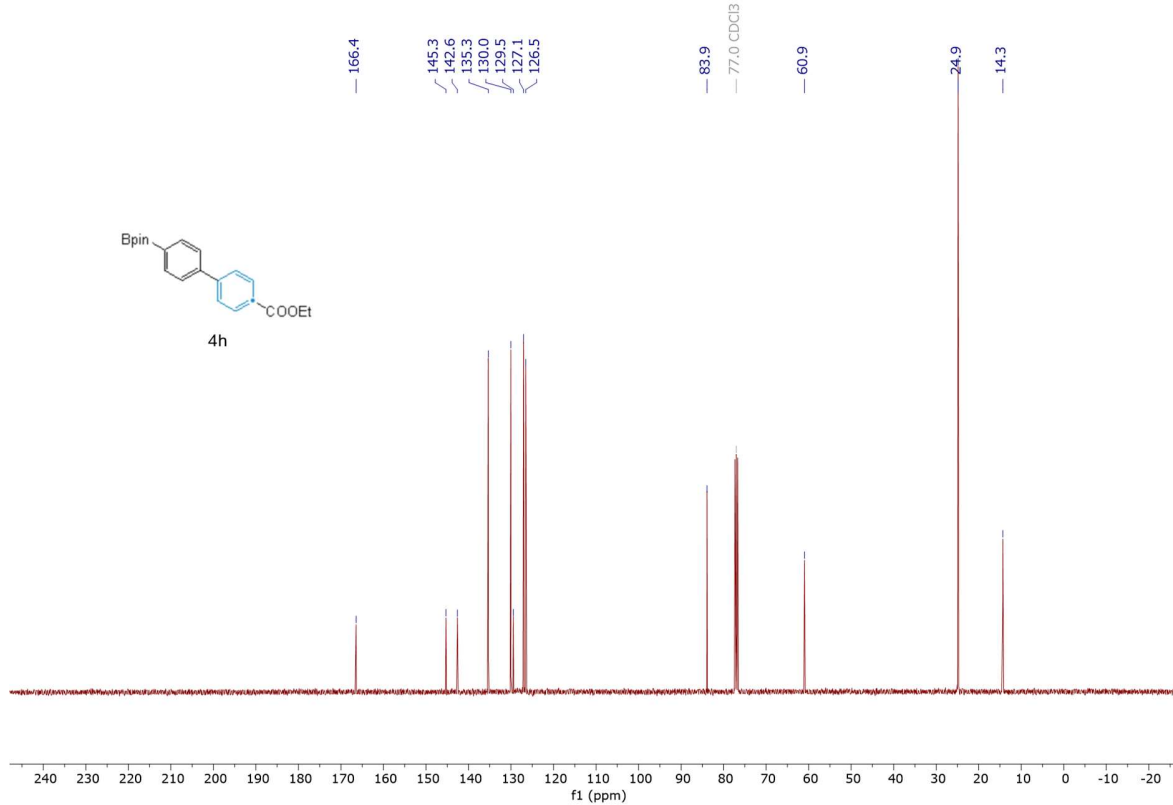
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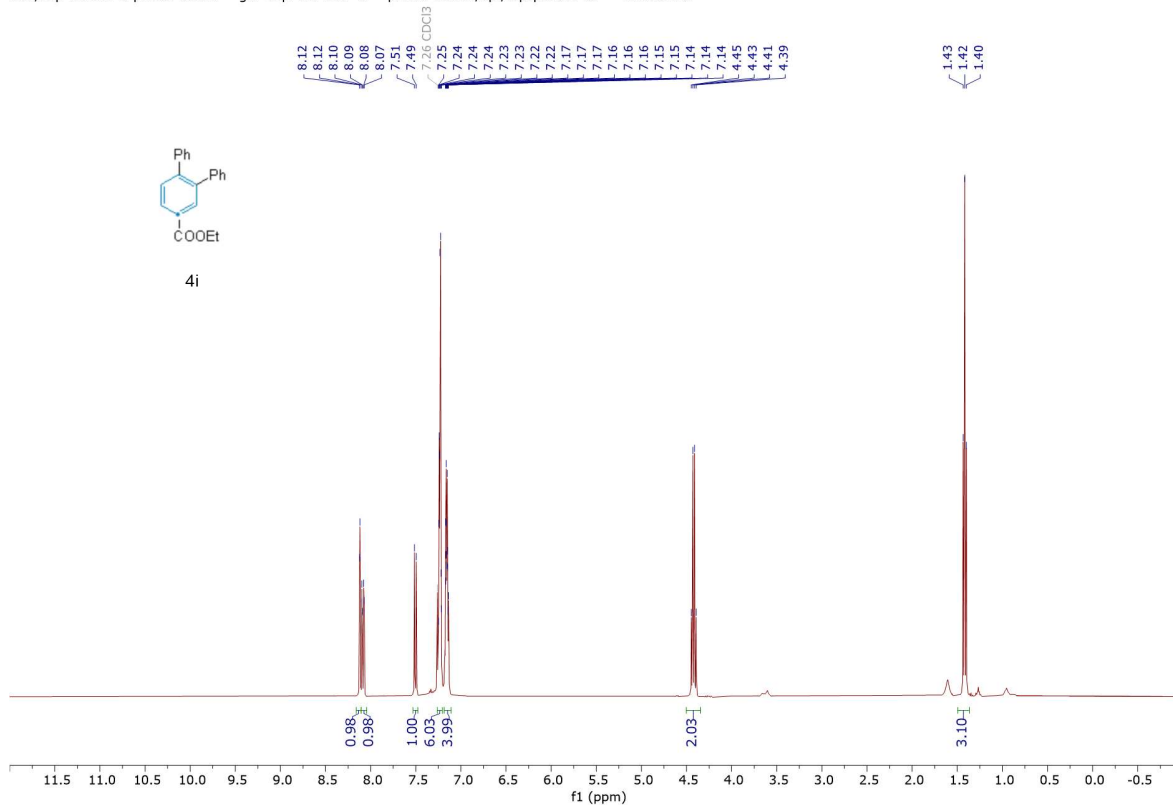
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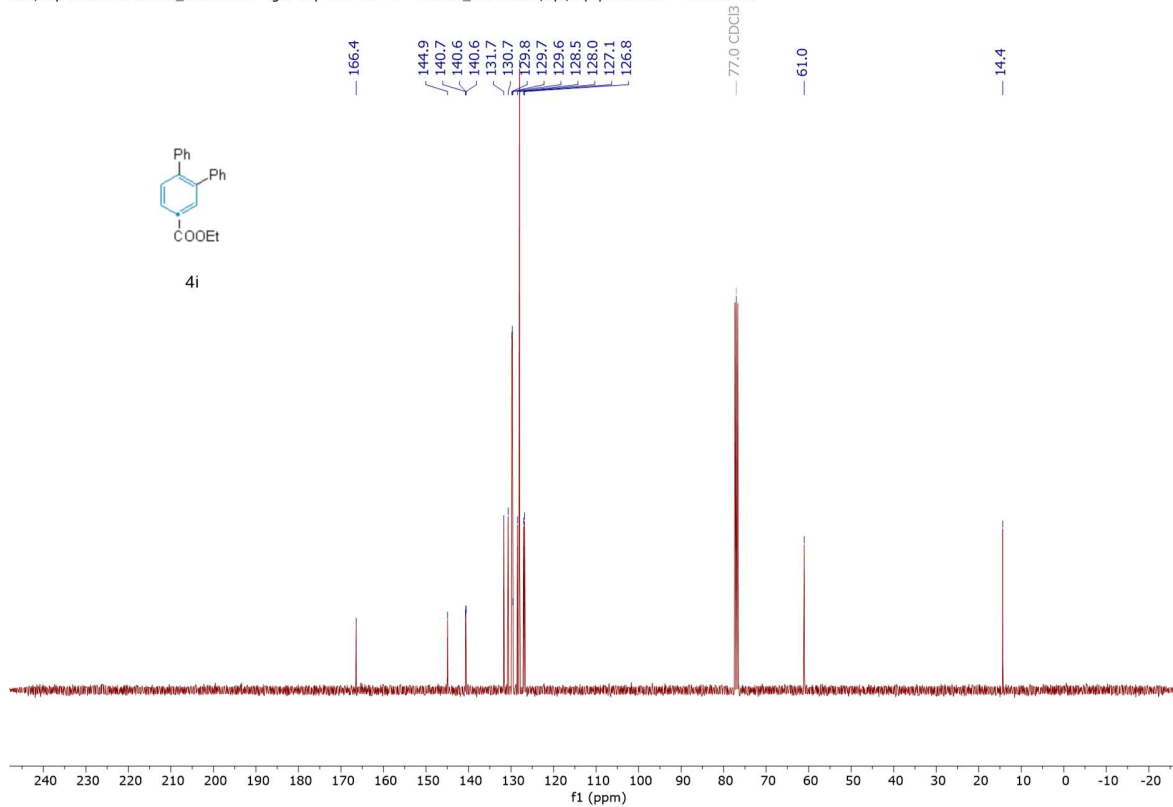
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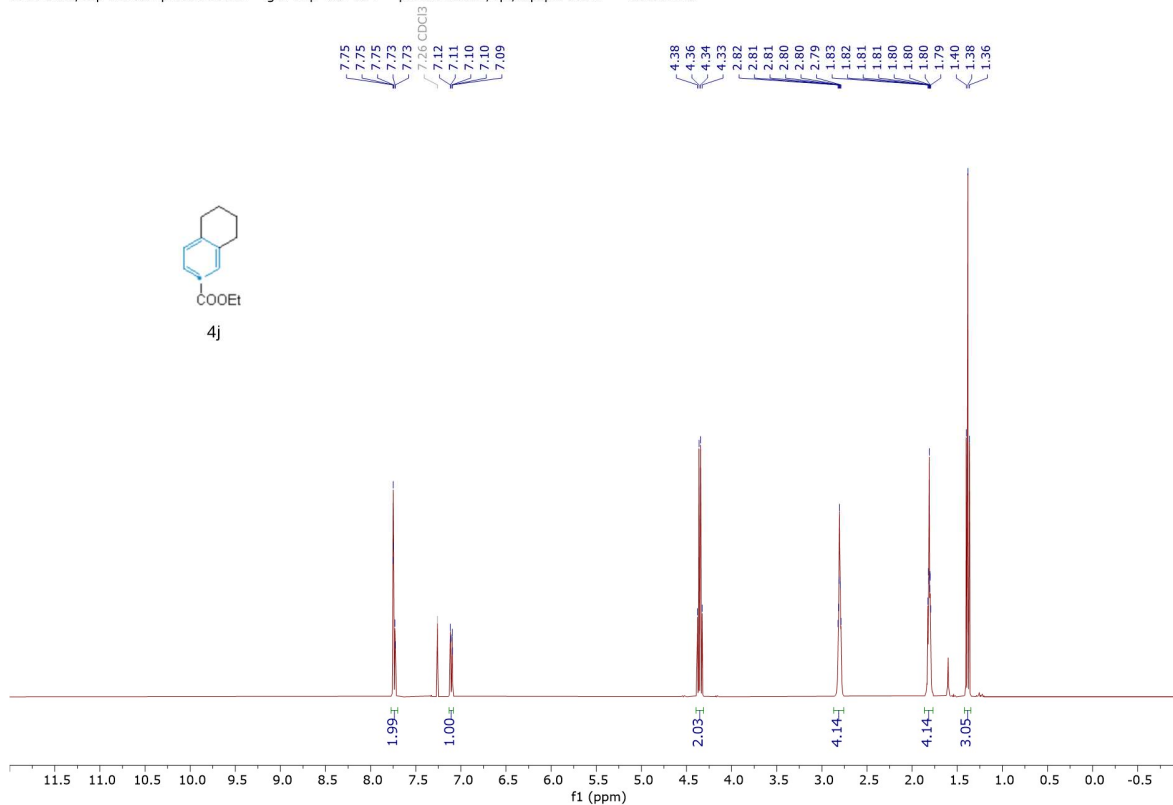
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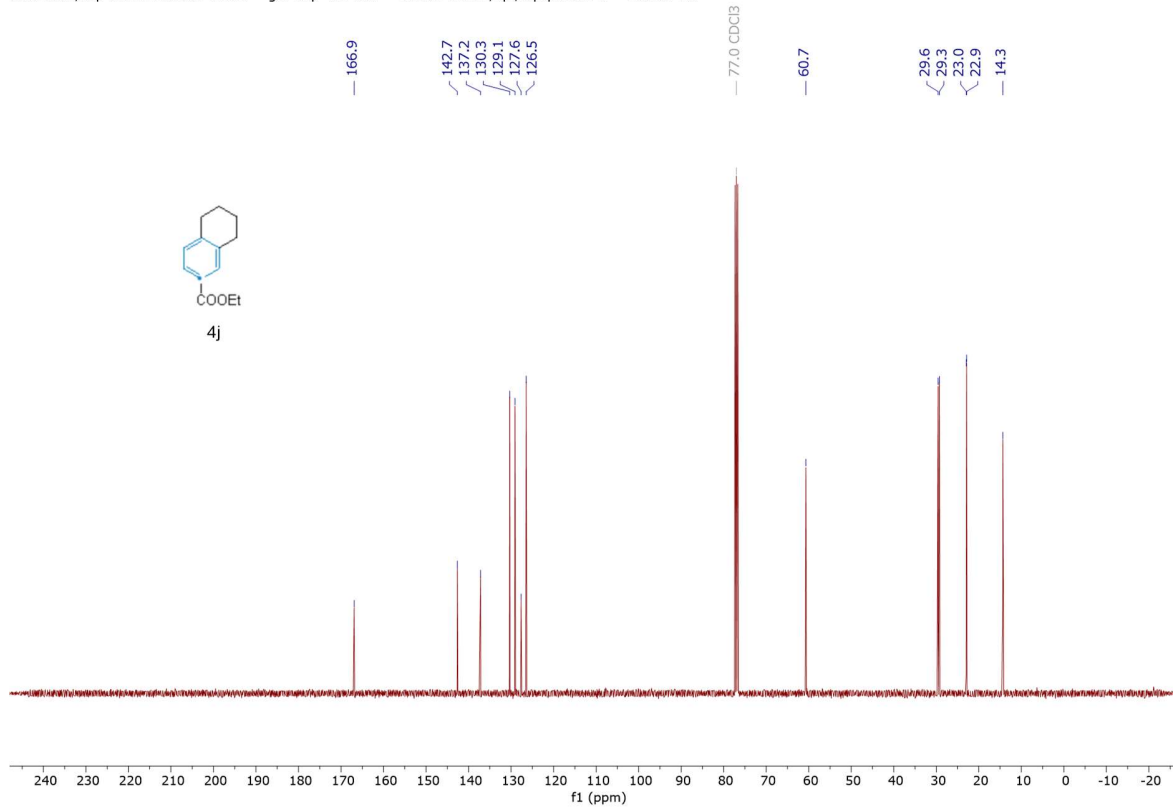
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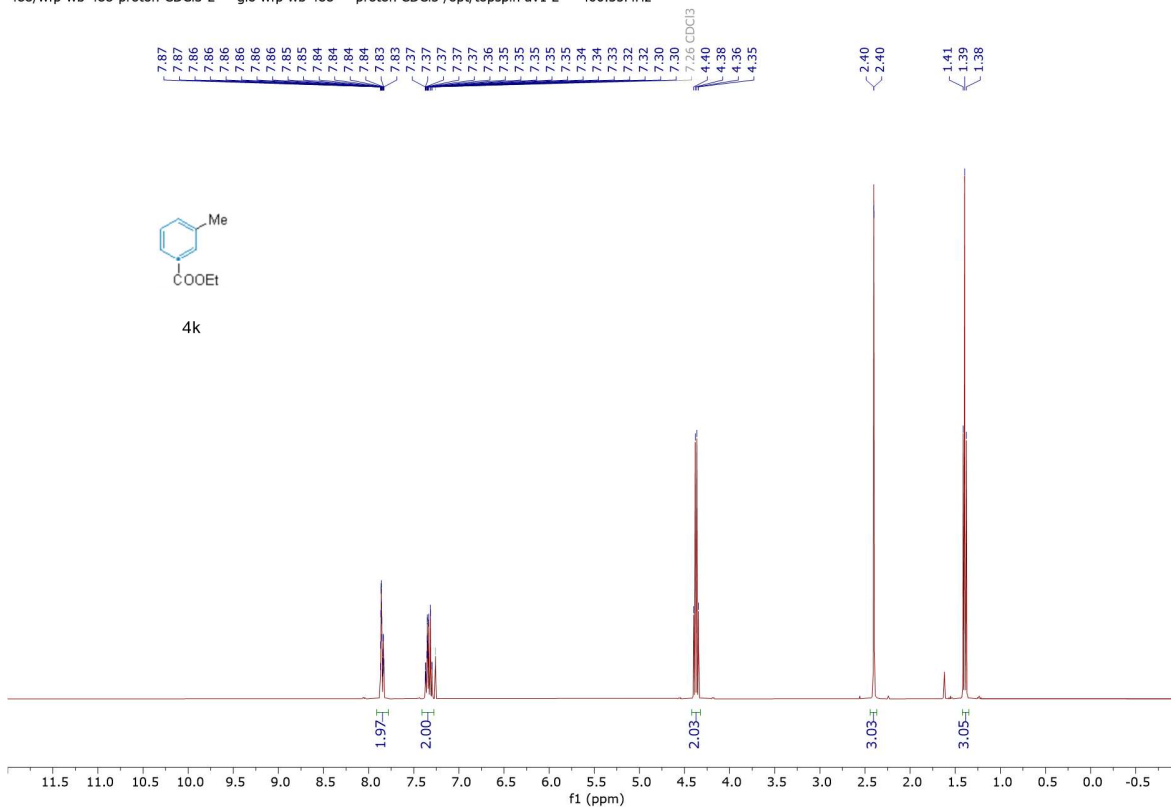
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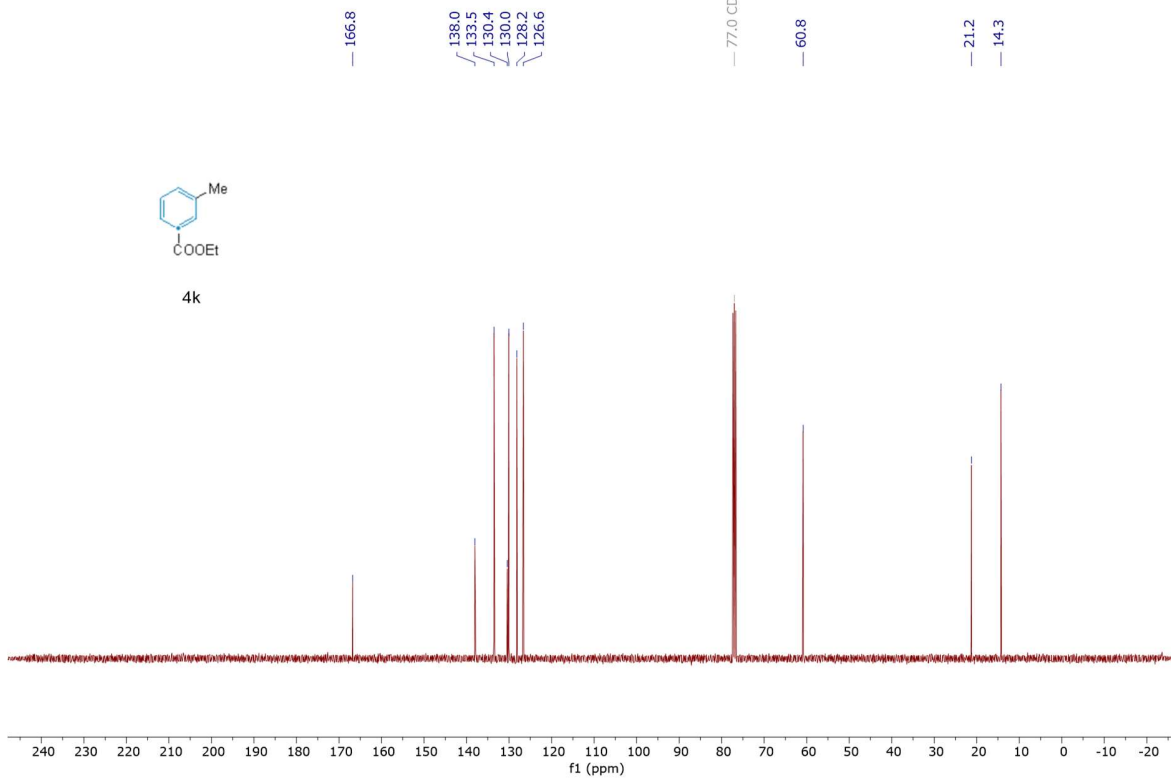
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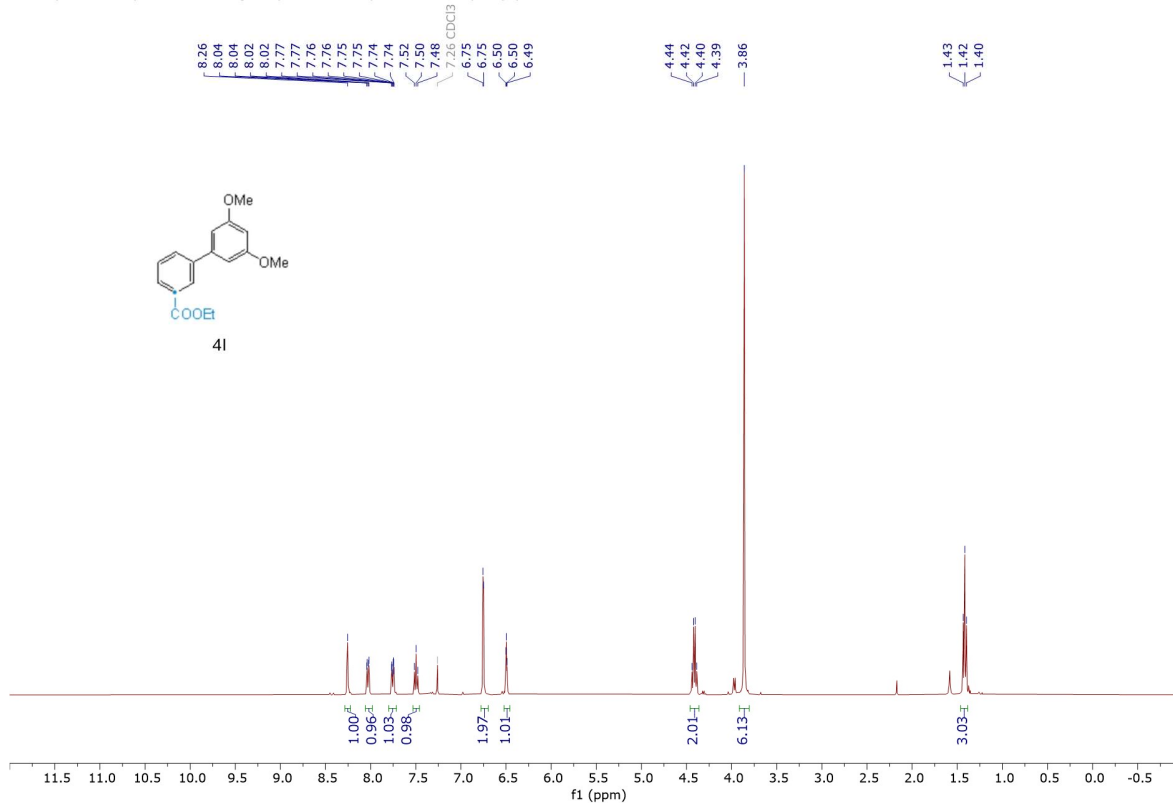
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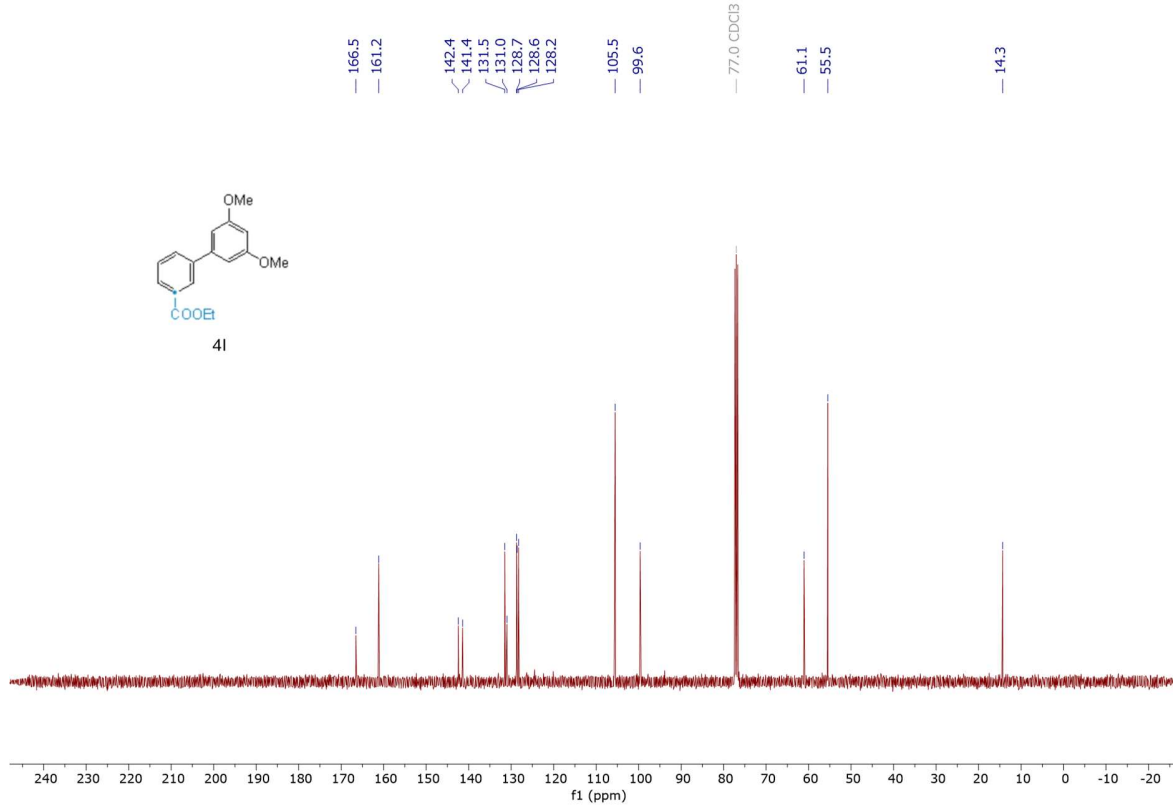
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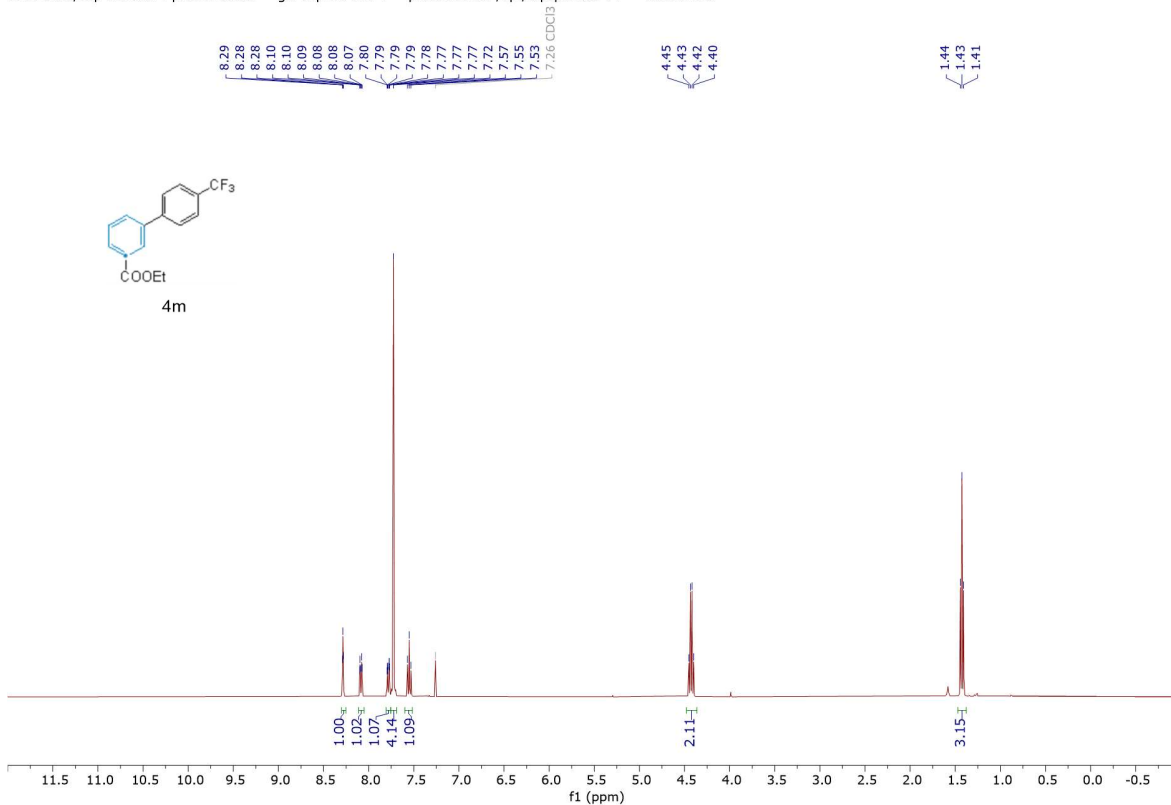
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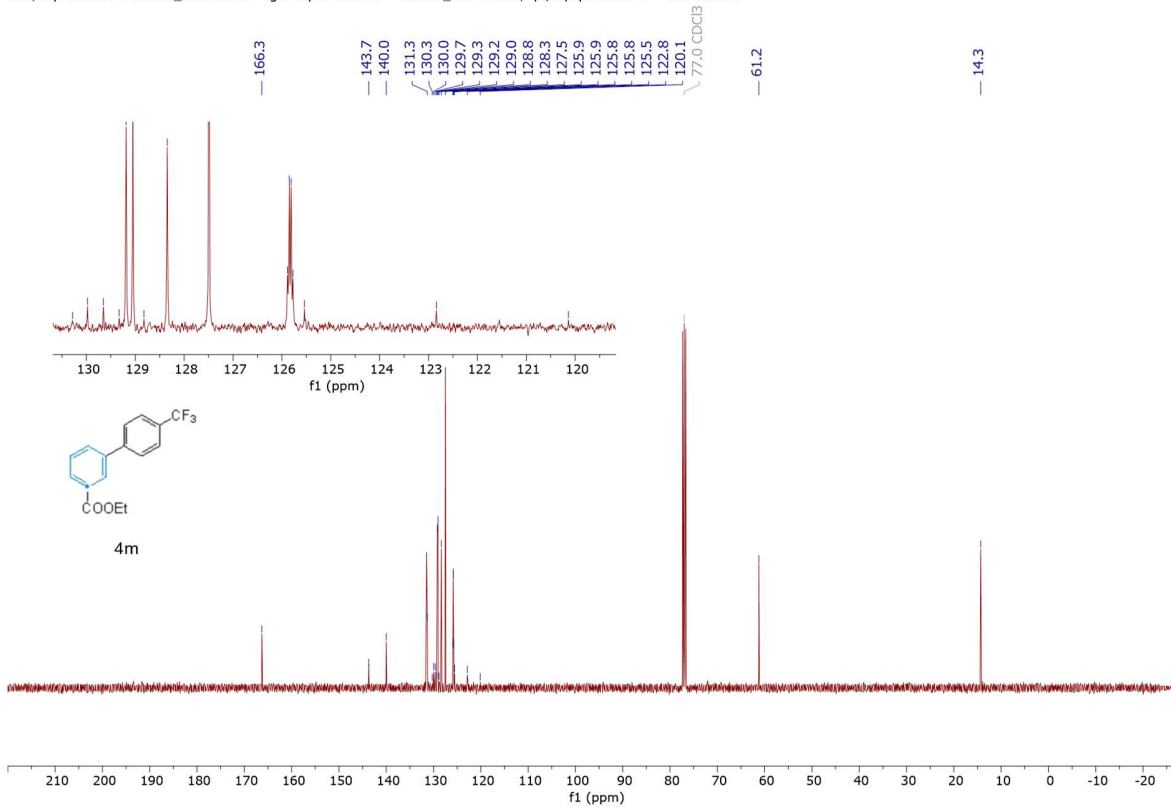
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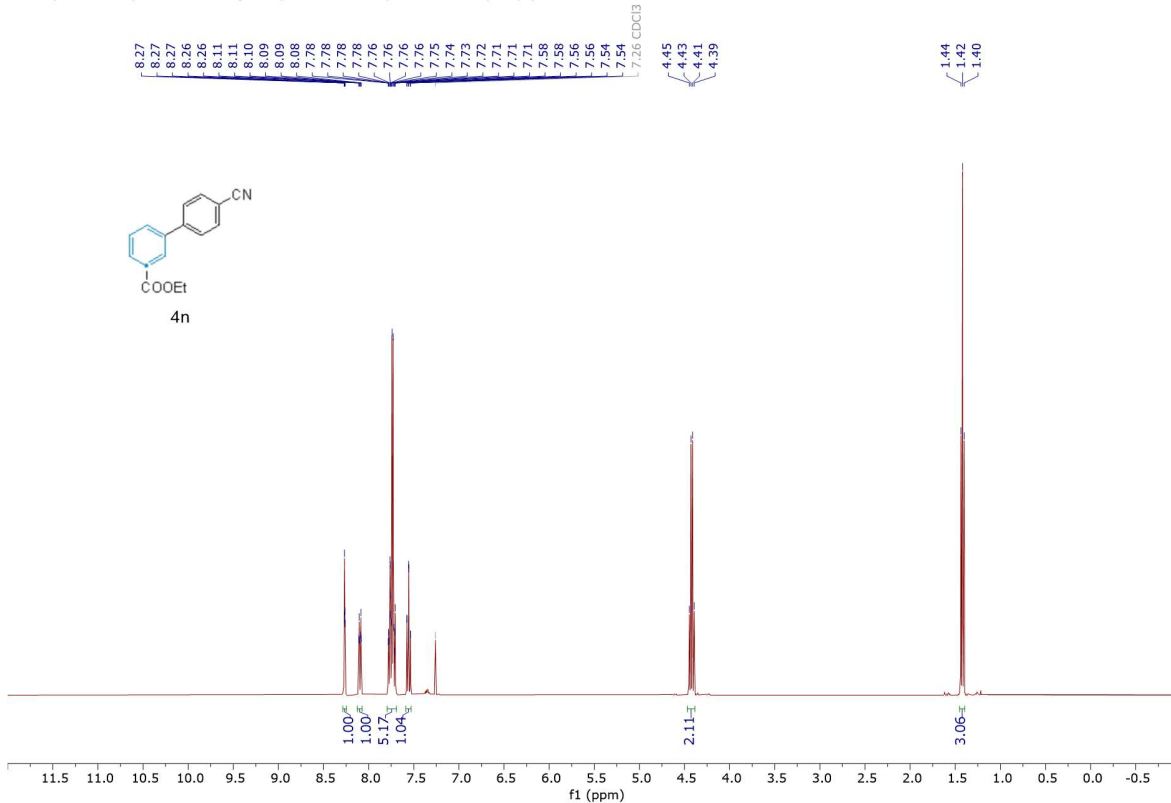
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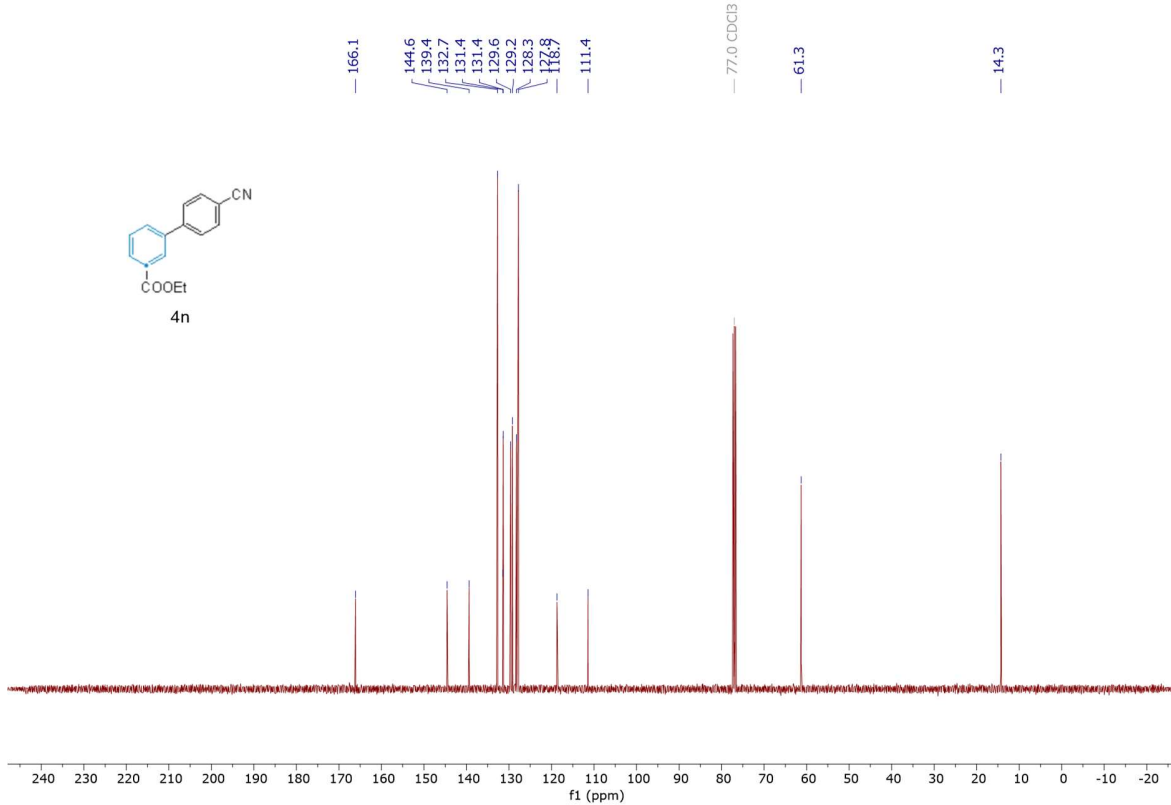
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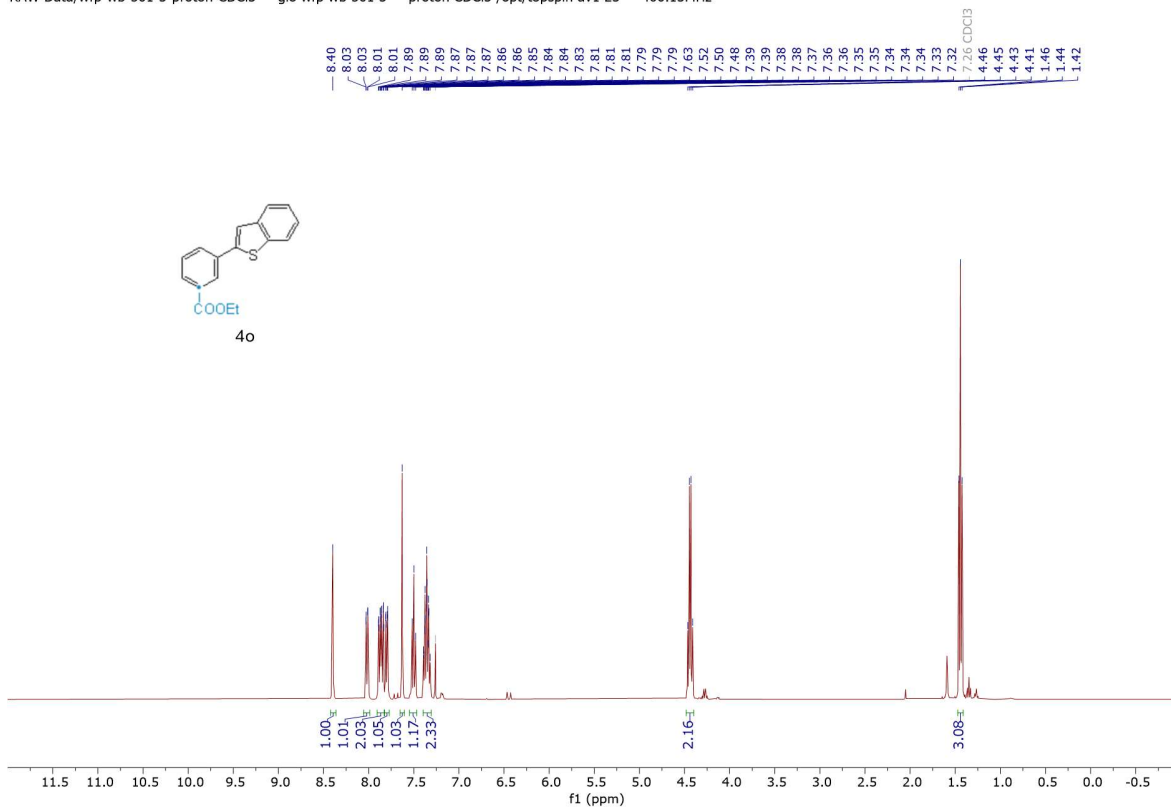
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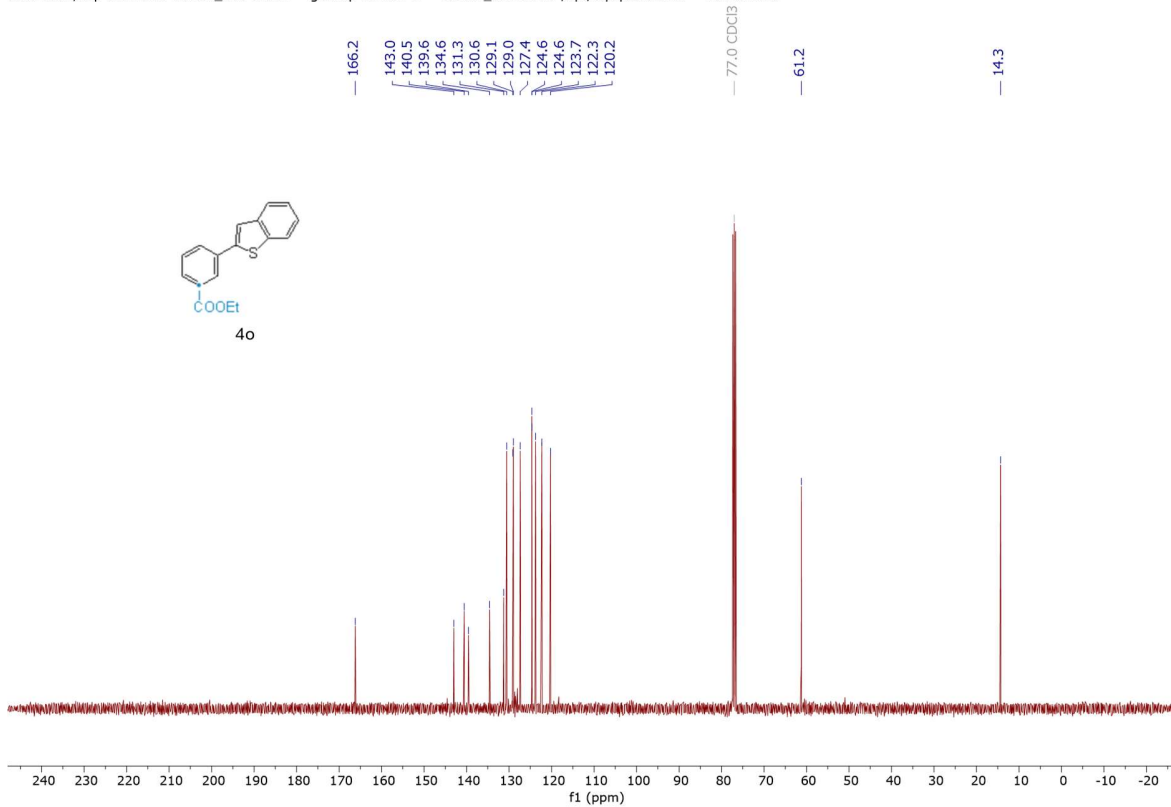
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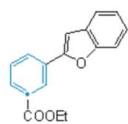
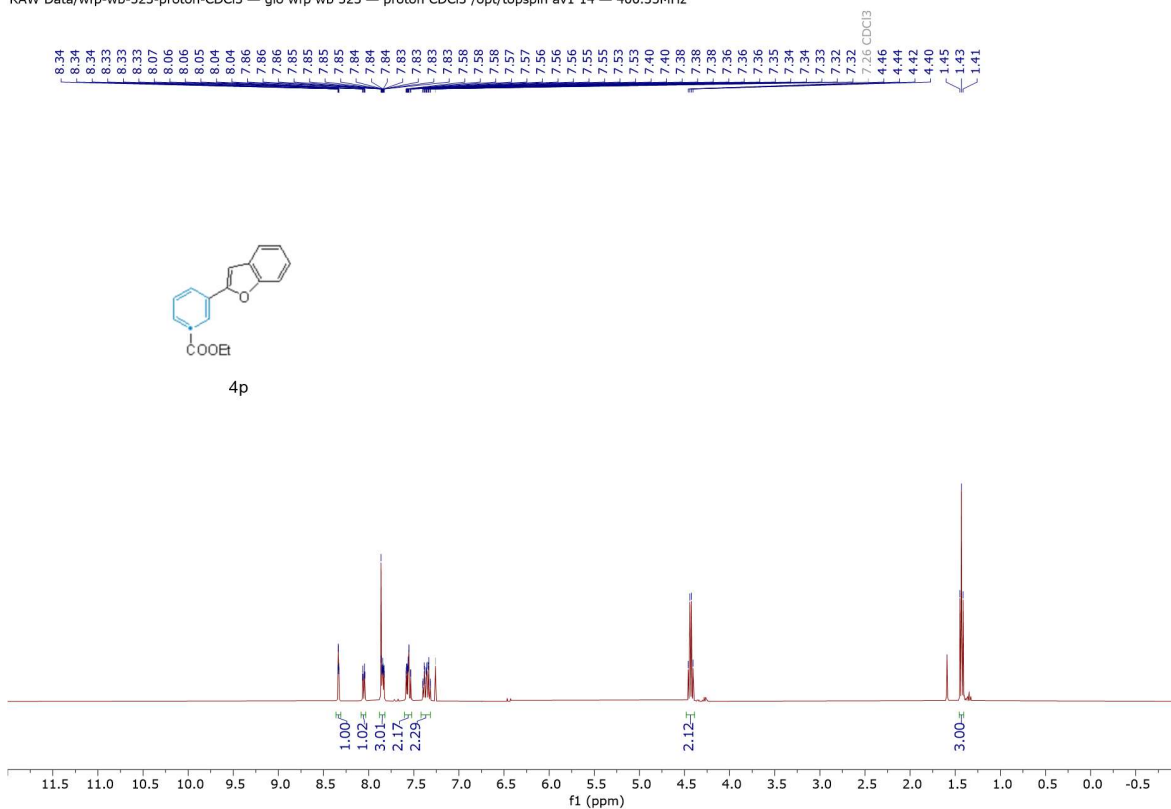
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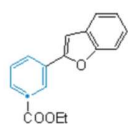
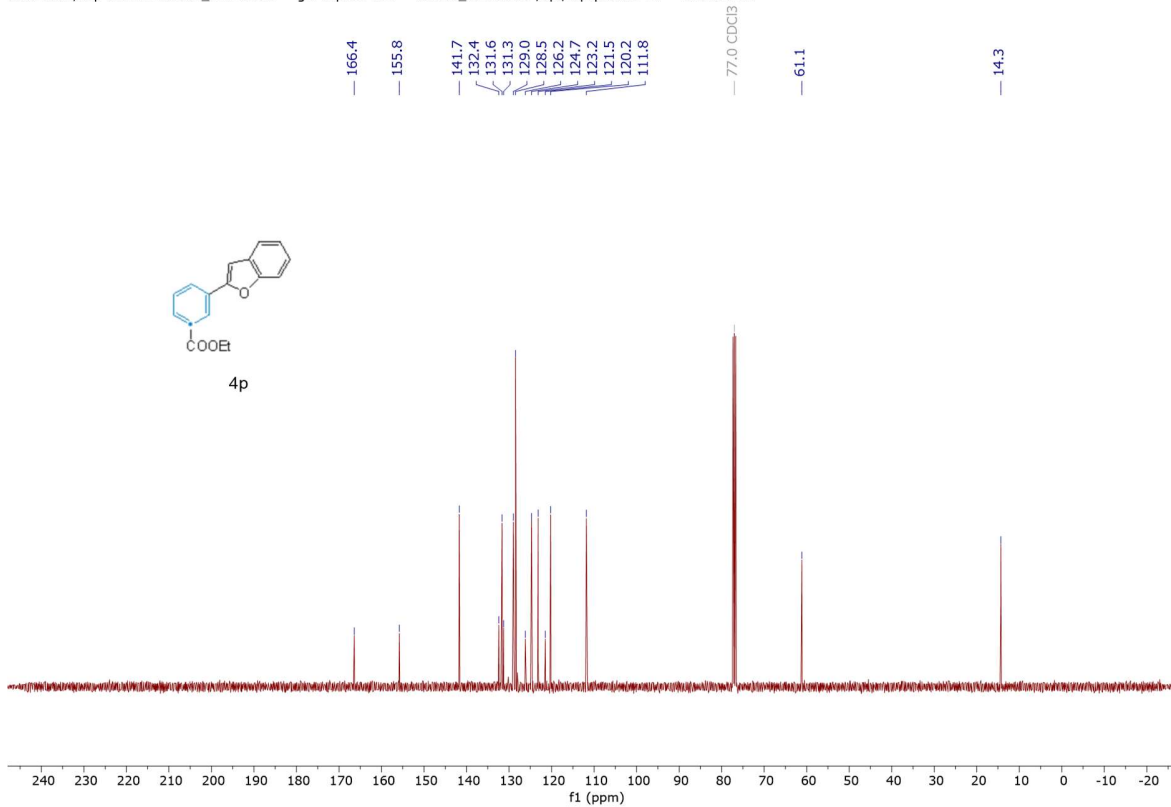


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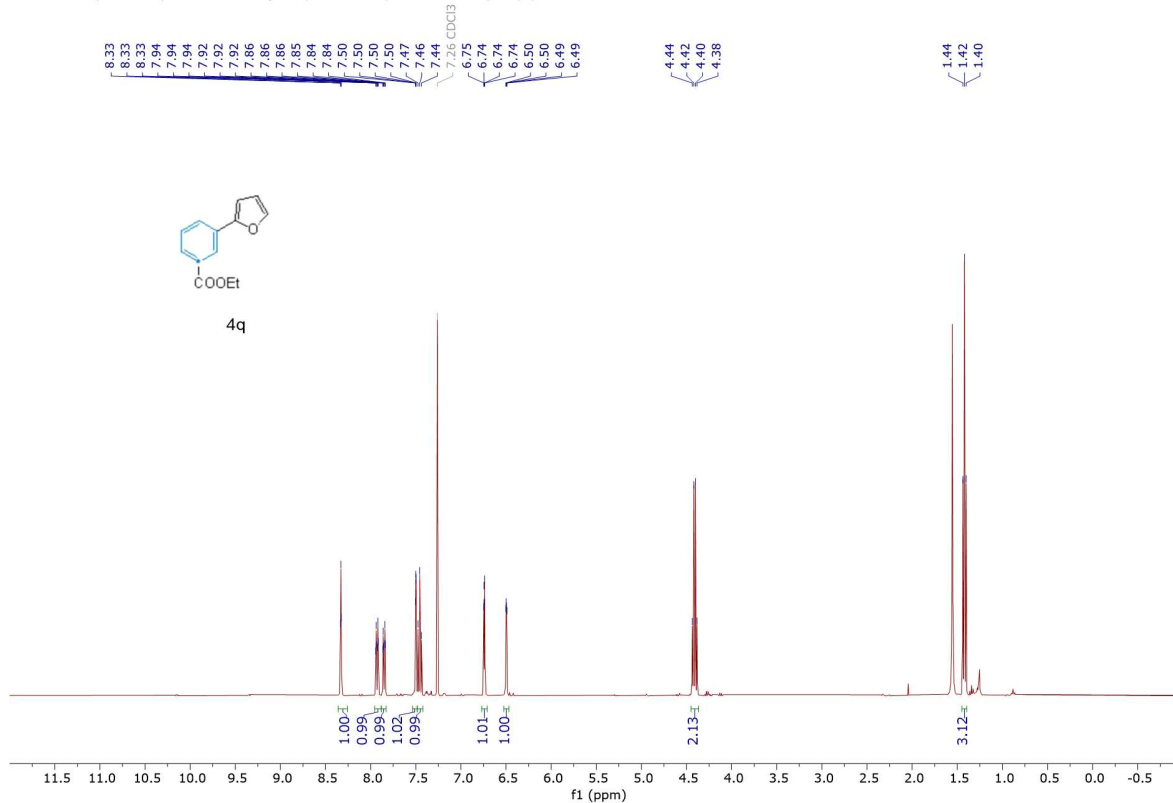
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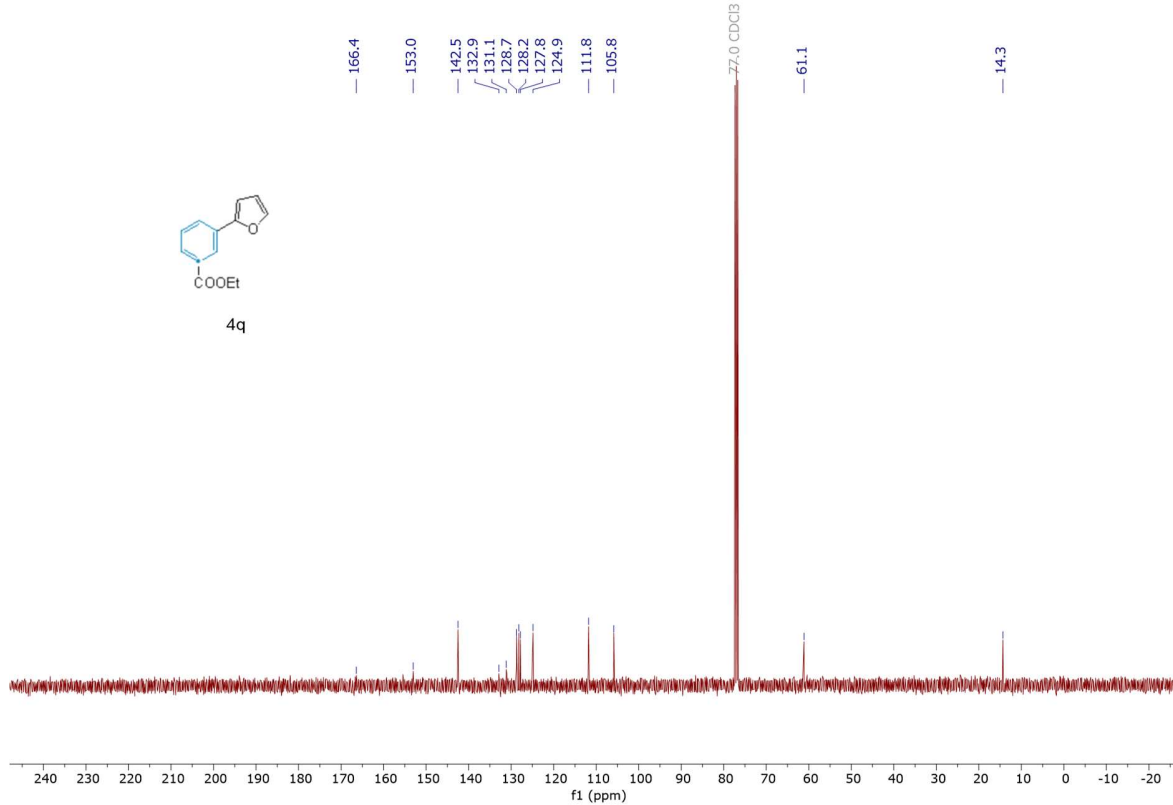


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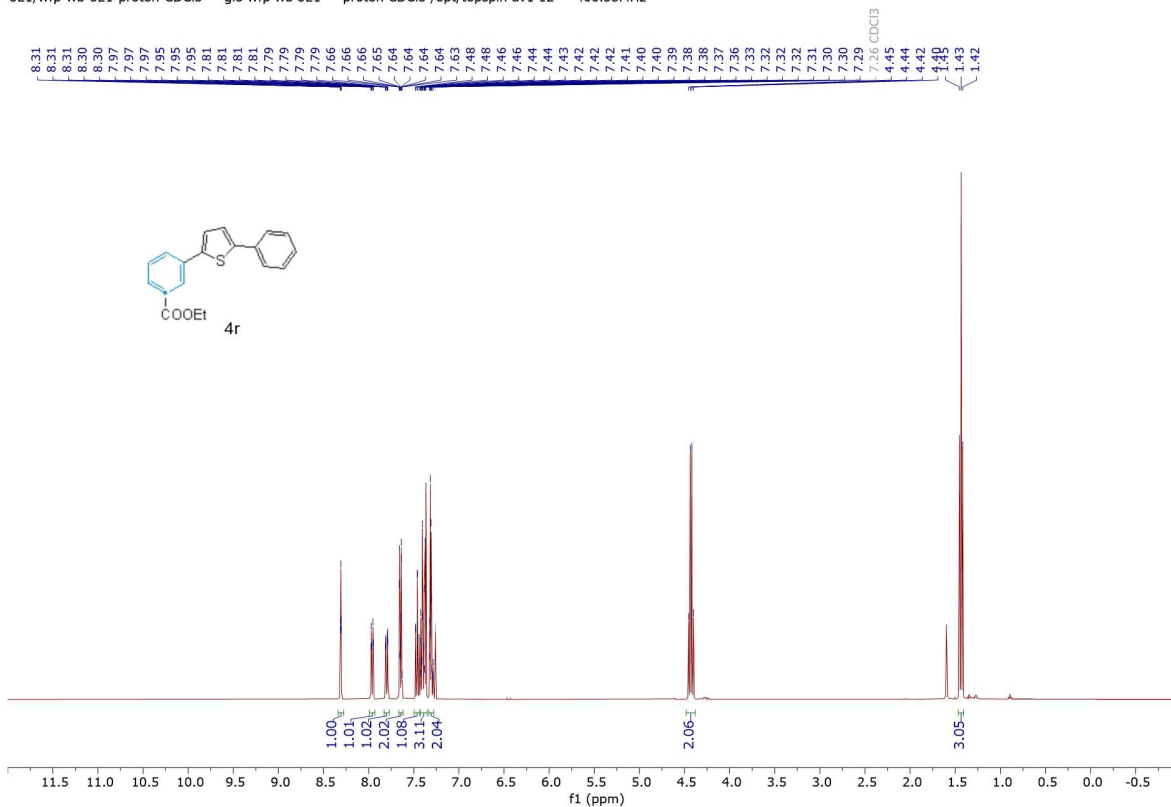
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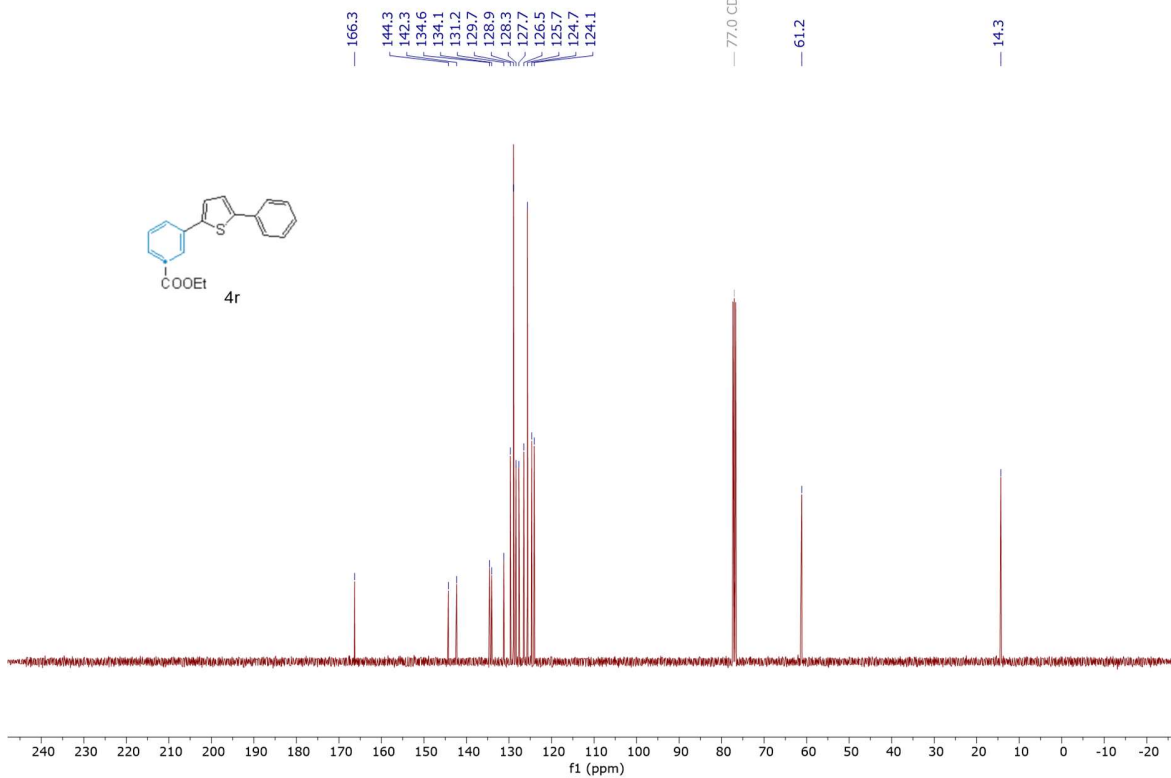
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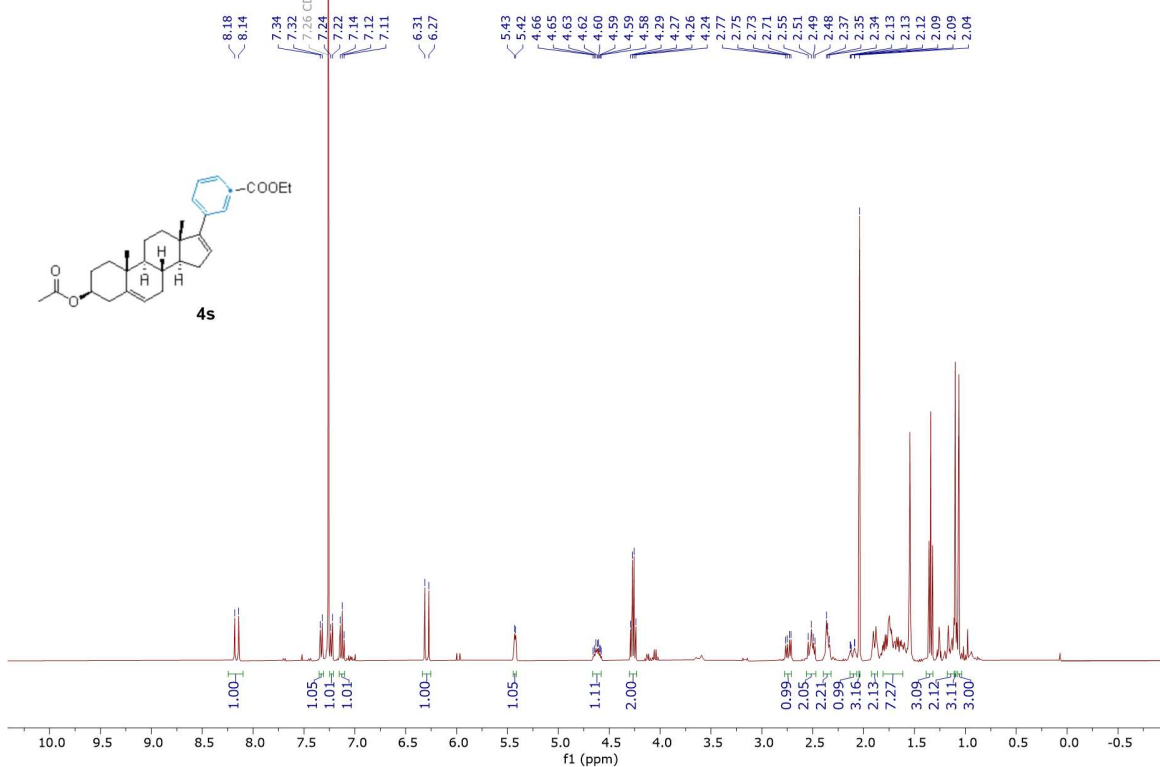
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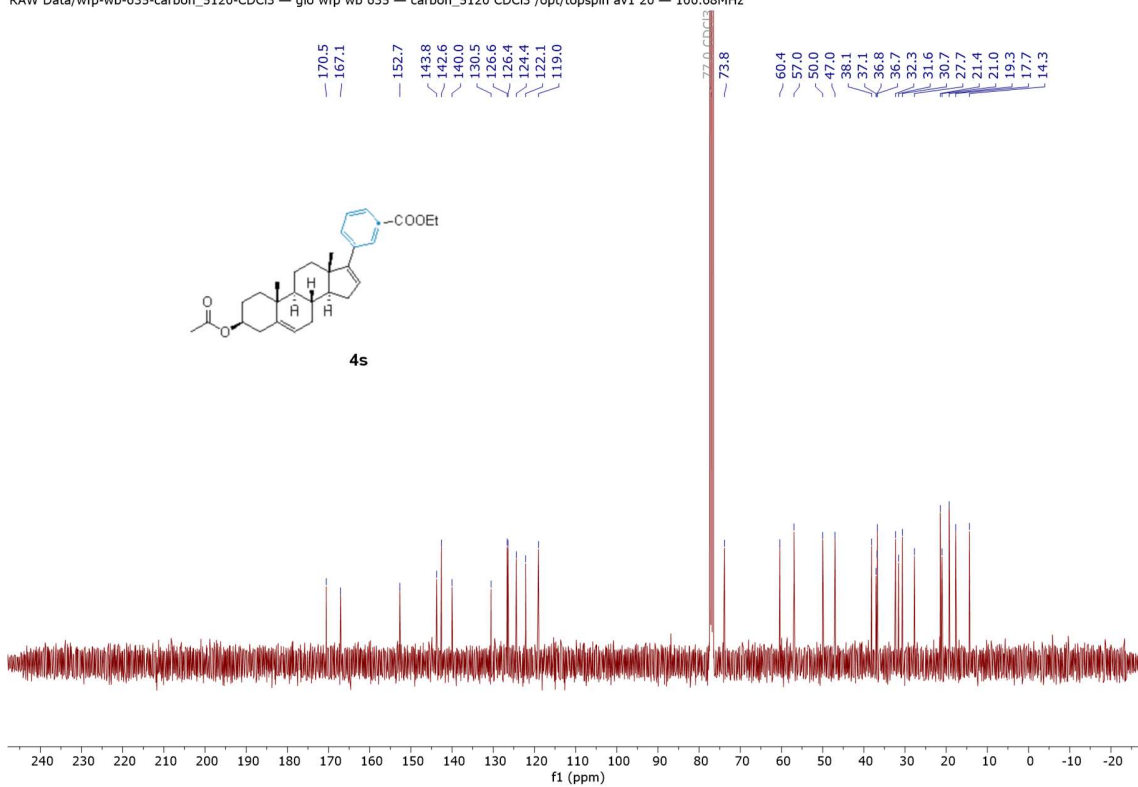
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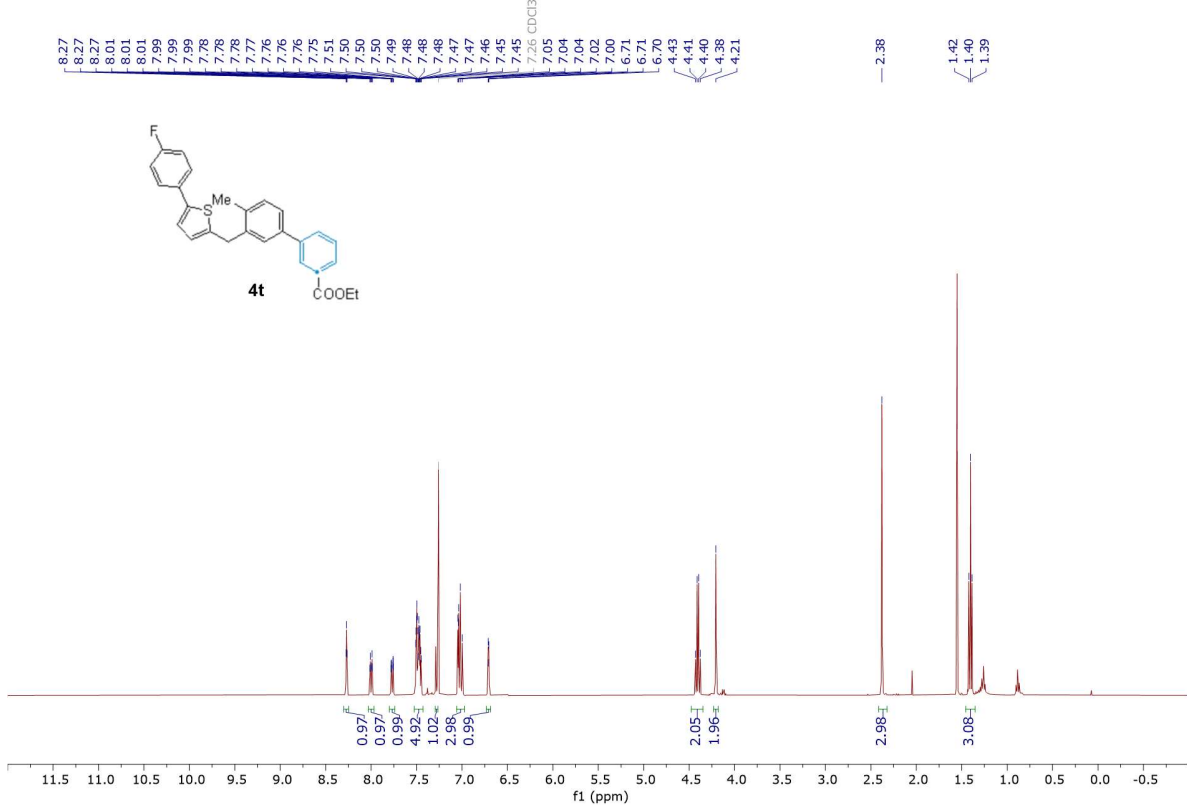
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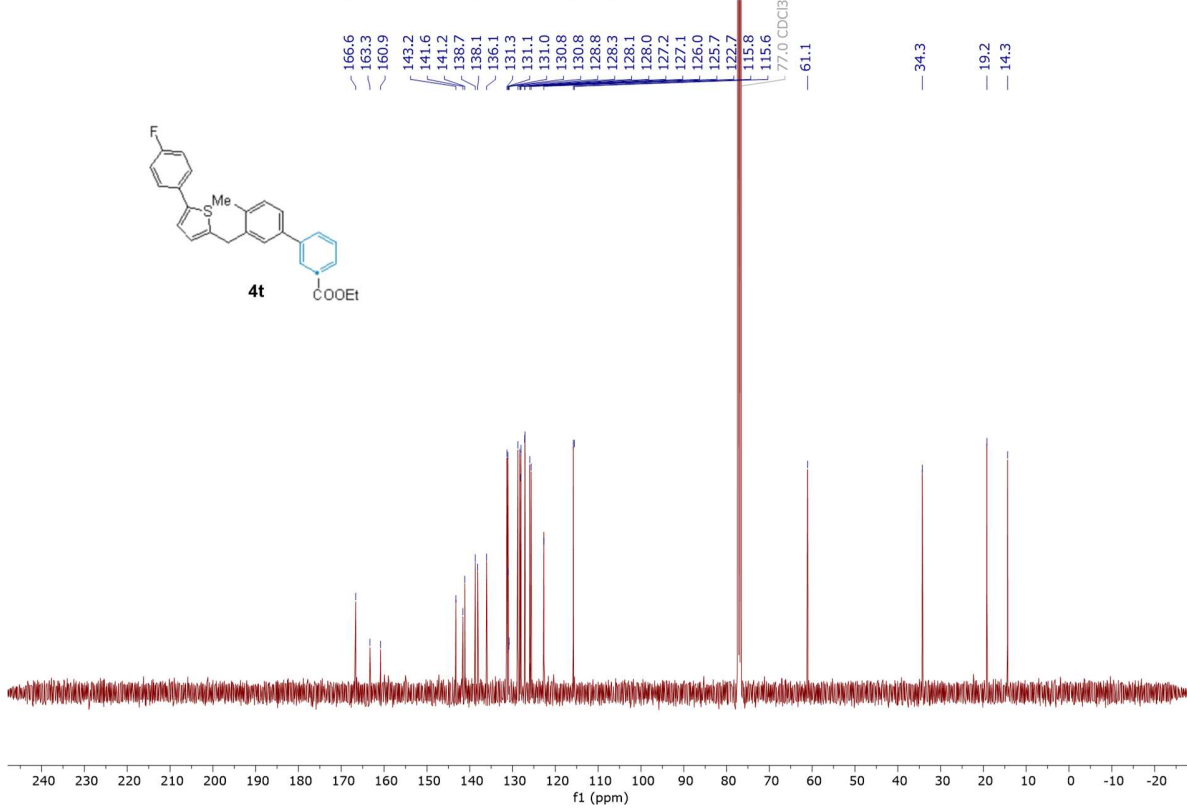
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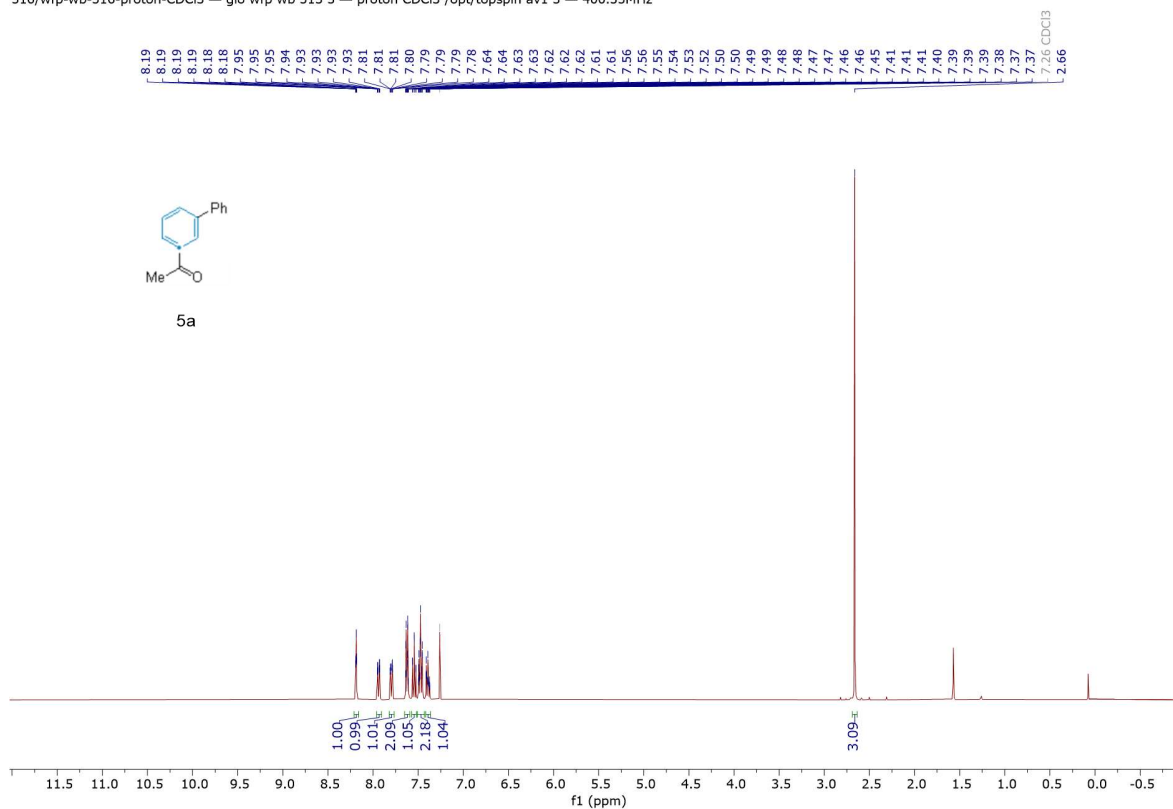
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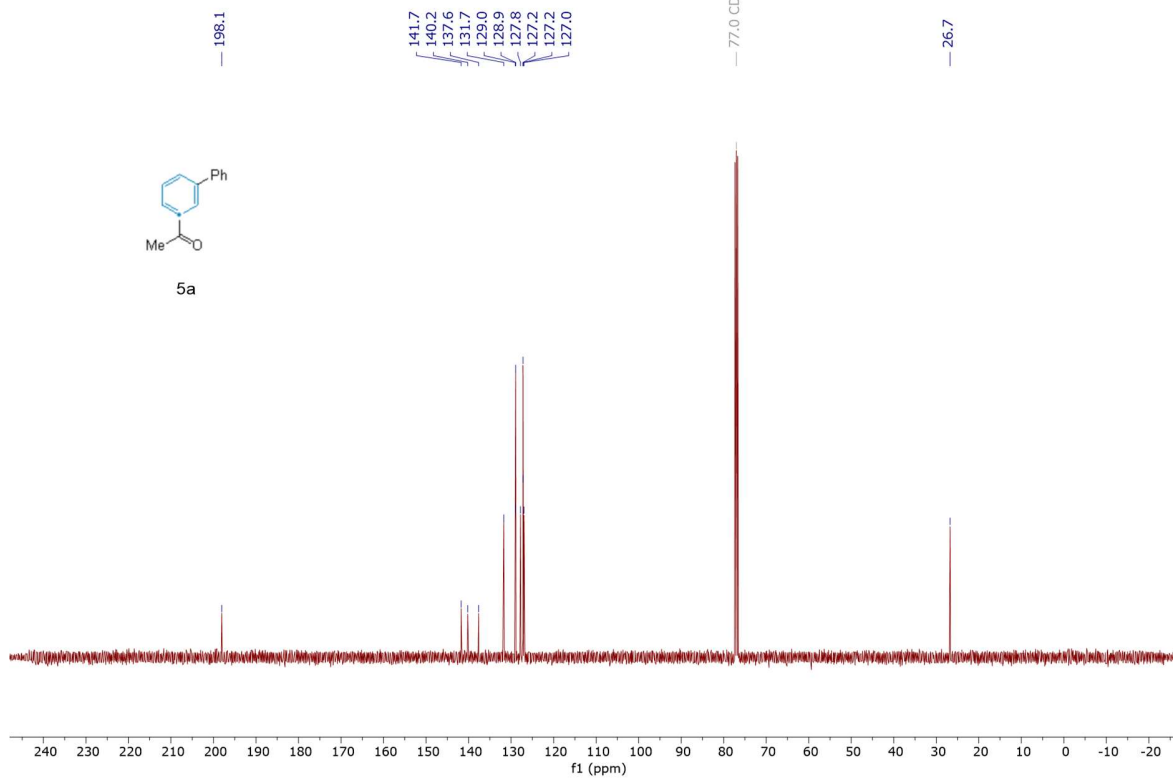
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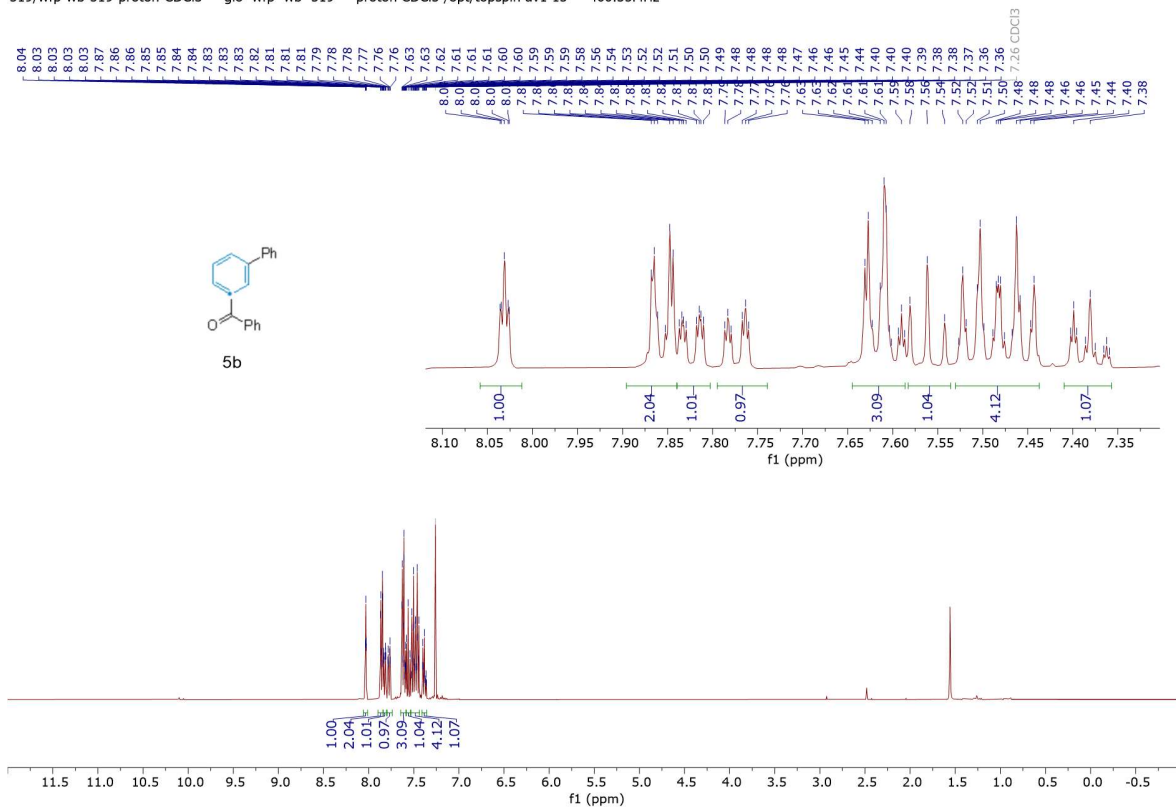
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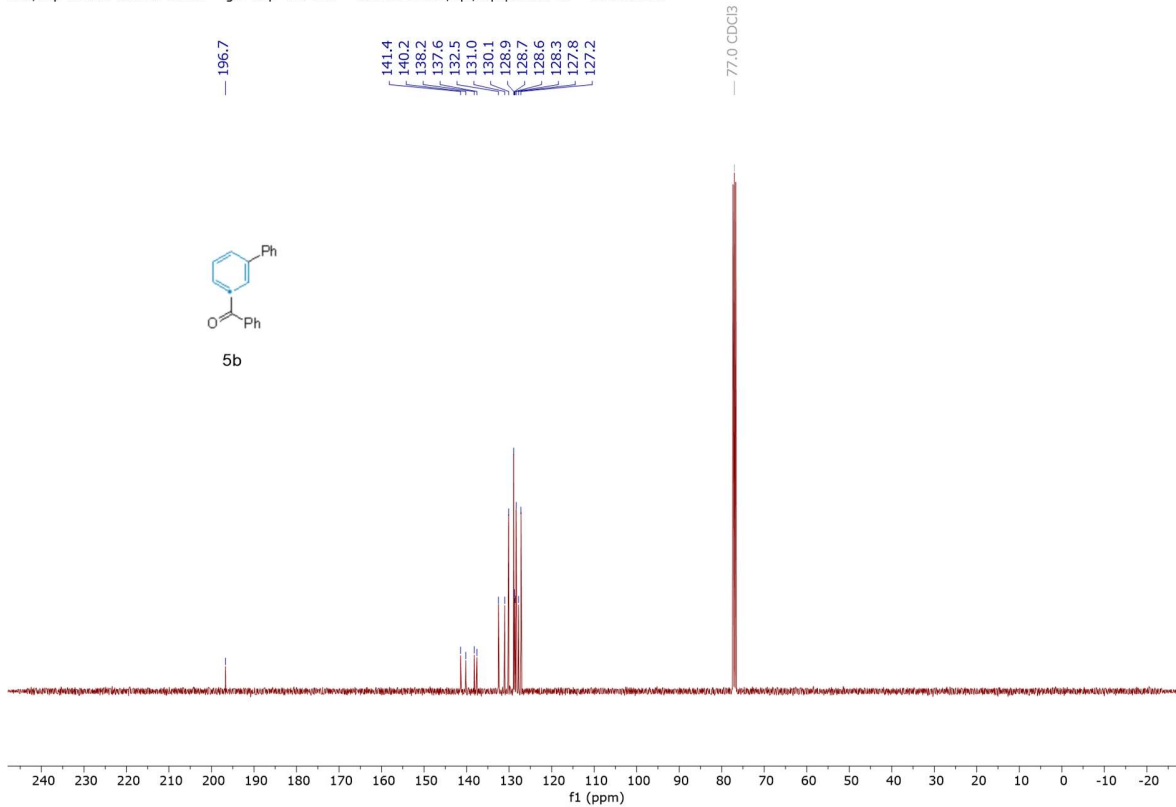
516/wfp-wb-516-carbon_256-CDCl3 — glo wfp wb 513 3 — carbon_256 CDCl3 /opt/topspin av1 3 — 100.68MHz



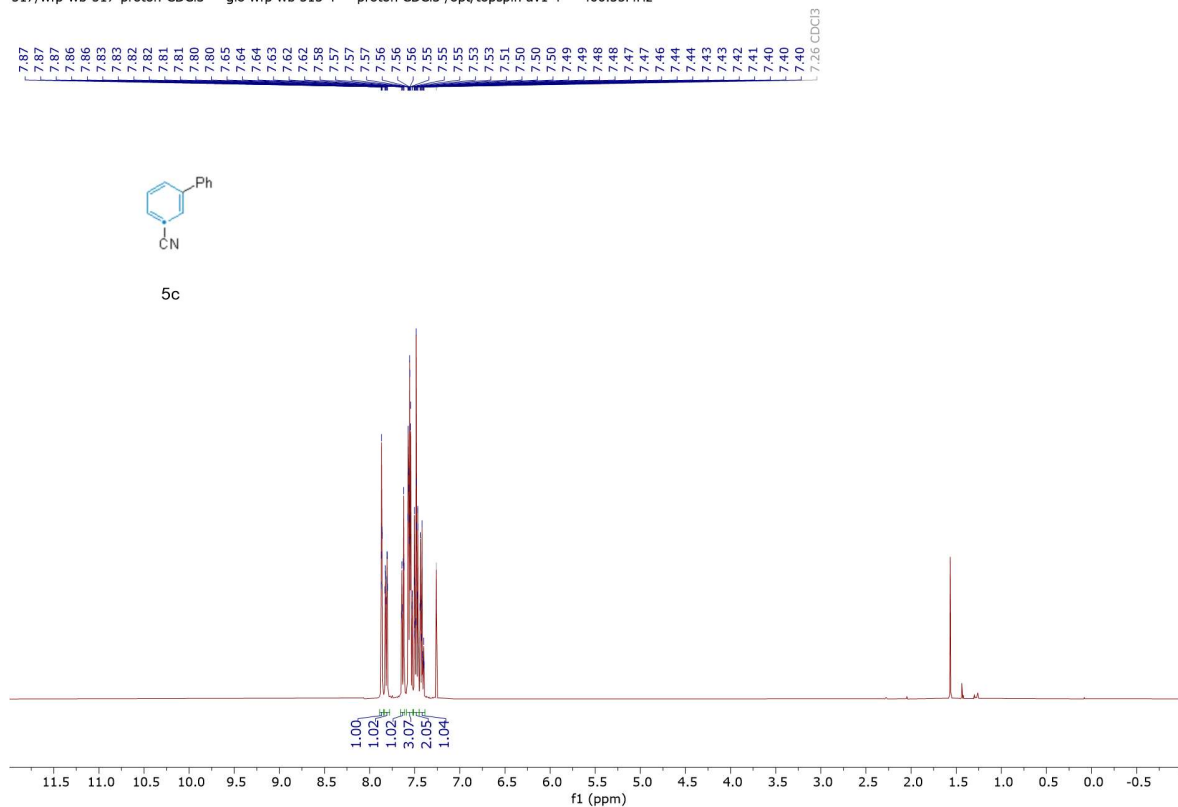
519/wfp-wb-519-proton-CDCl3 — glo wfp wb 519 — proton CDCl3 /opt/topspin av1 15 — 400.35MHz



519/wfp-wb-519-carbon-CDCl3 — glo wfp wb 519 — carbon CDCl3 /opt/topspin av1 15 — 100.68MHz

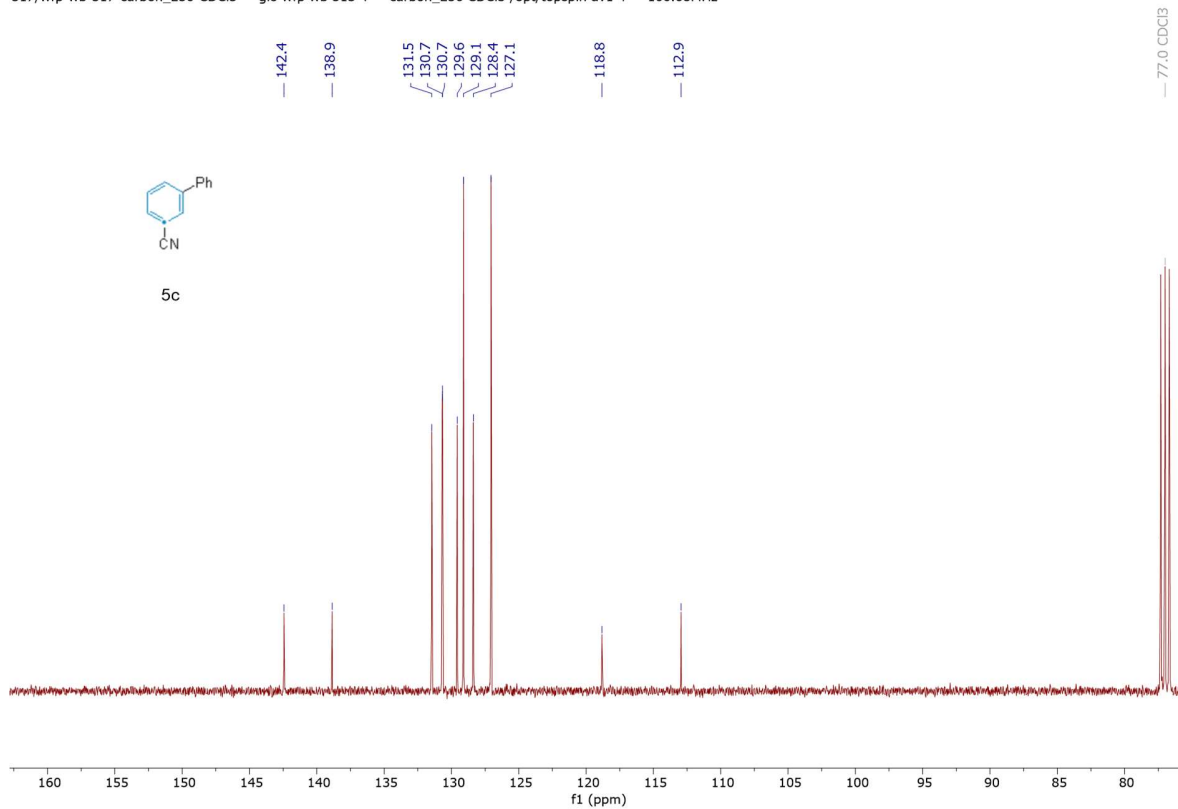


517/wfp-wb-517-proton-CDCl3 — glo wfp wb 513 4 — proton CDCl3 /opt/topspin av1 4 — 400.35MHz



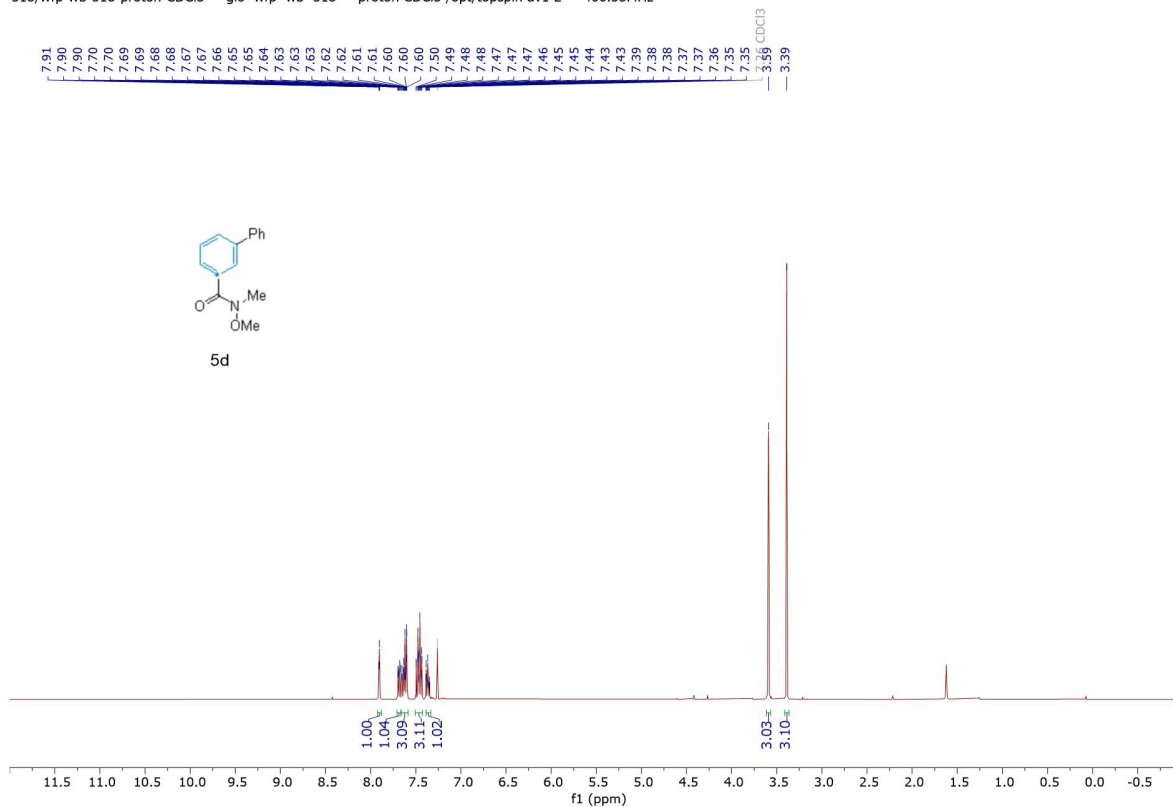
5c

517/wfp-wb-517-carbon_256-CDCl3 — glo wfp wb 513 4 — carbon_256 CDCl3 /opt/topspin av1 4 — 100.68MHz

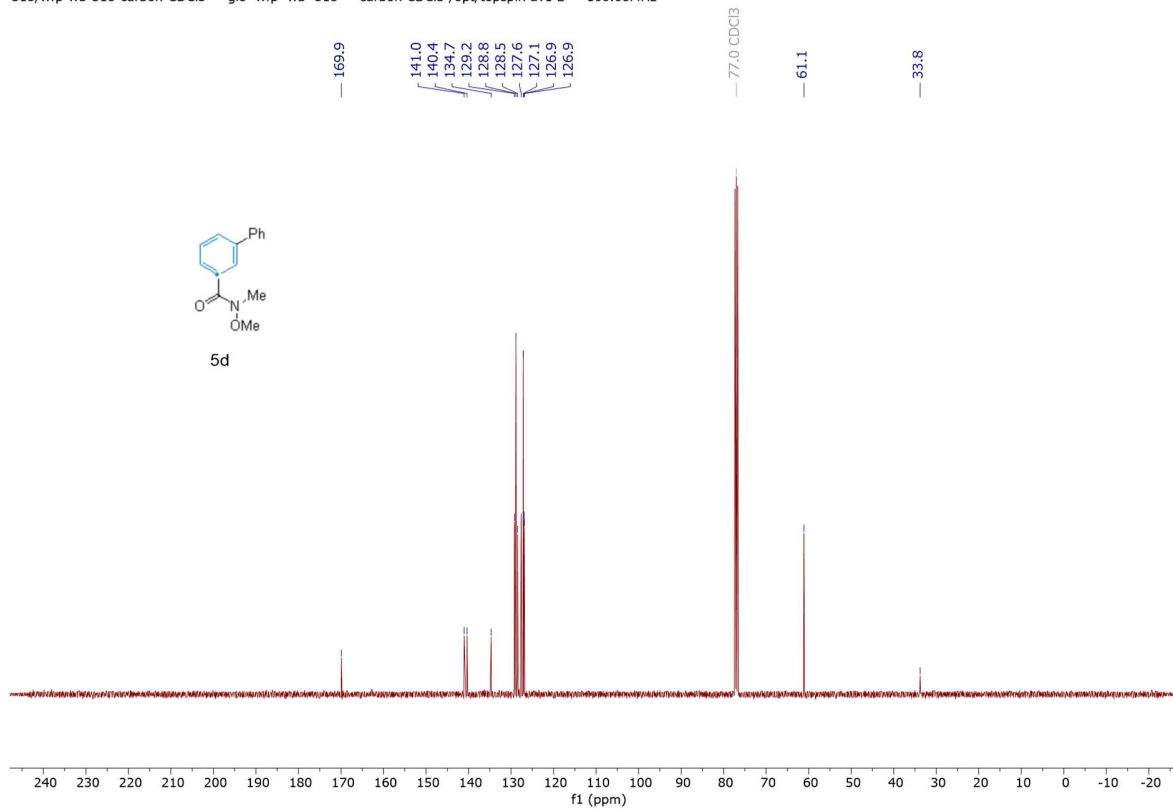


5c

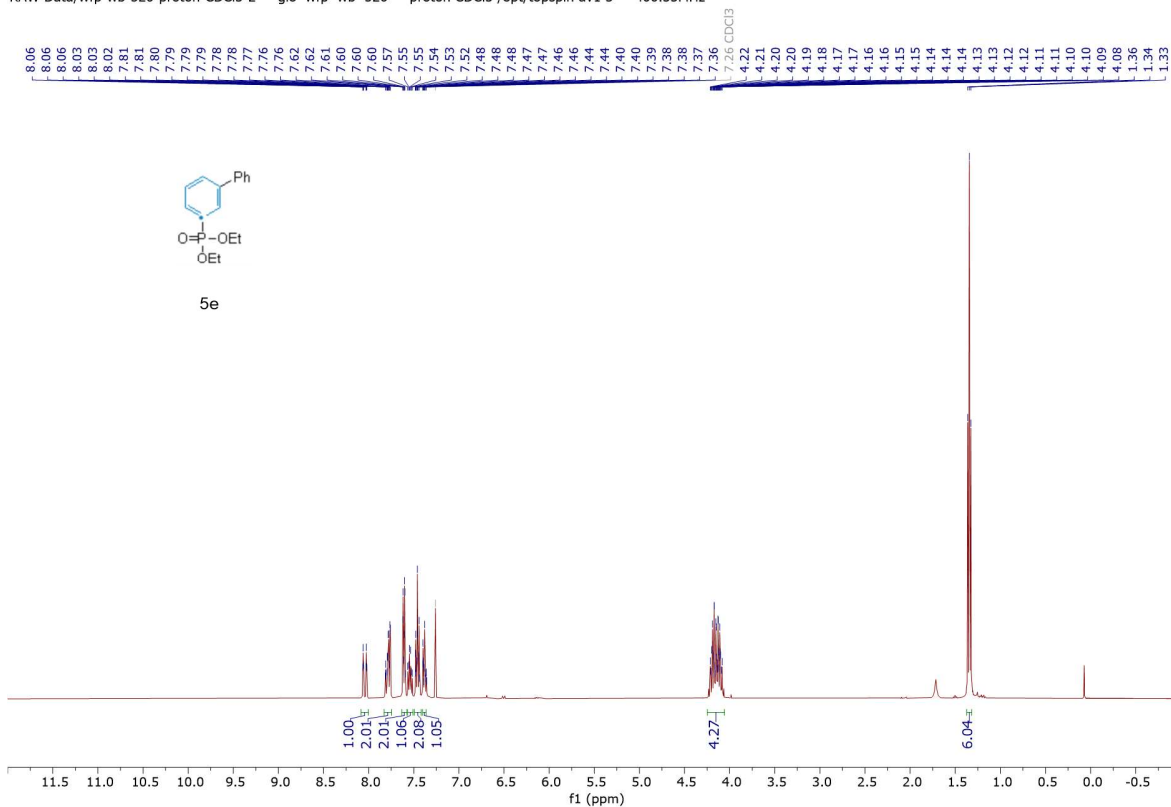
518/wfp-wb-518-proton-CDCl3 — glo wfp wb 518 — proton CDCl3 /opt/topspin av1 2 — 400.35MHz



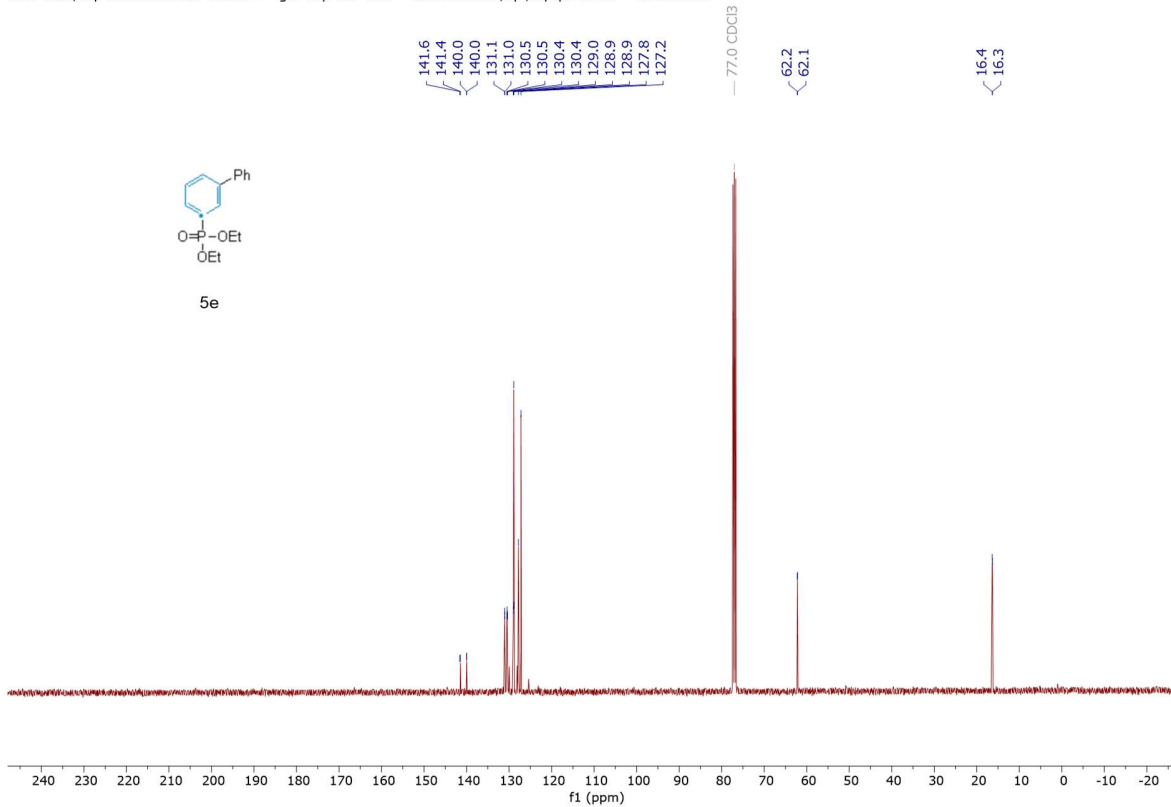
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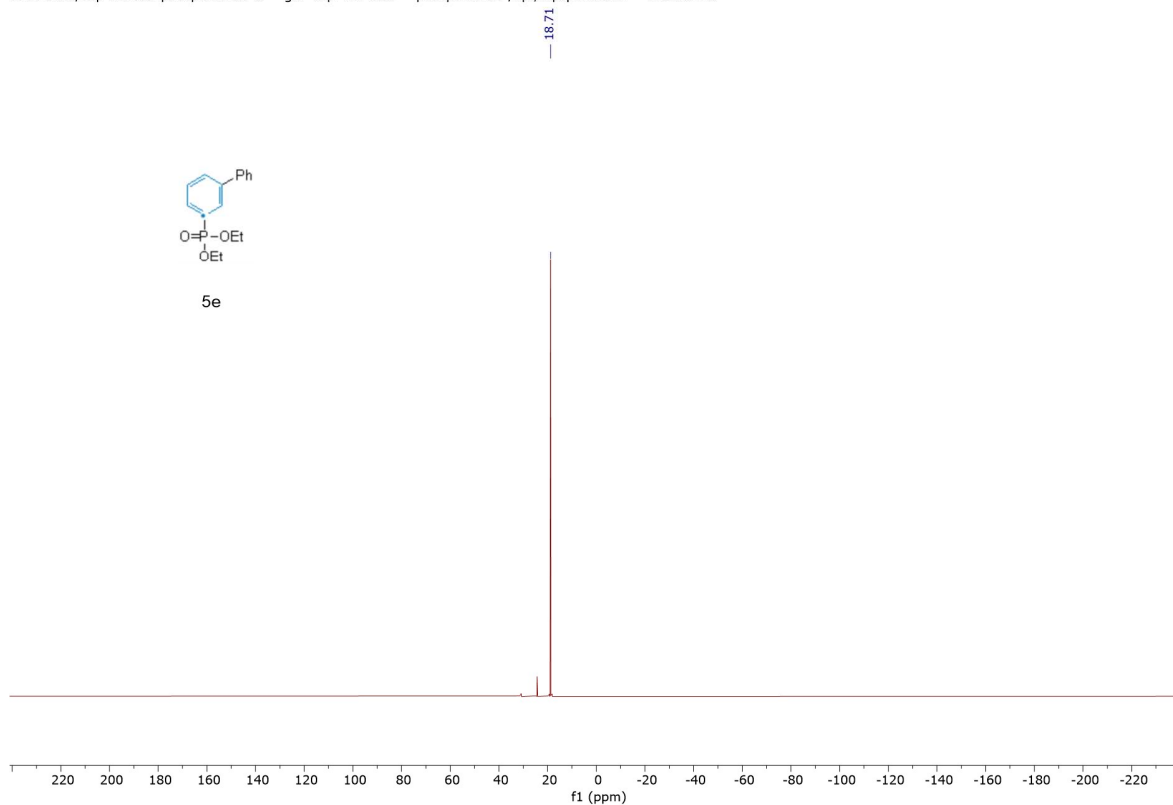
RAW Data/wfp-wb-520-proton-CDCl3-2 — glo wfp wb 520 — proton CDCl3 /opt/topspin av1 3 — 400.35MHz



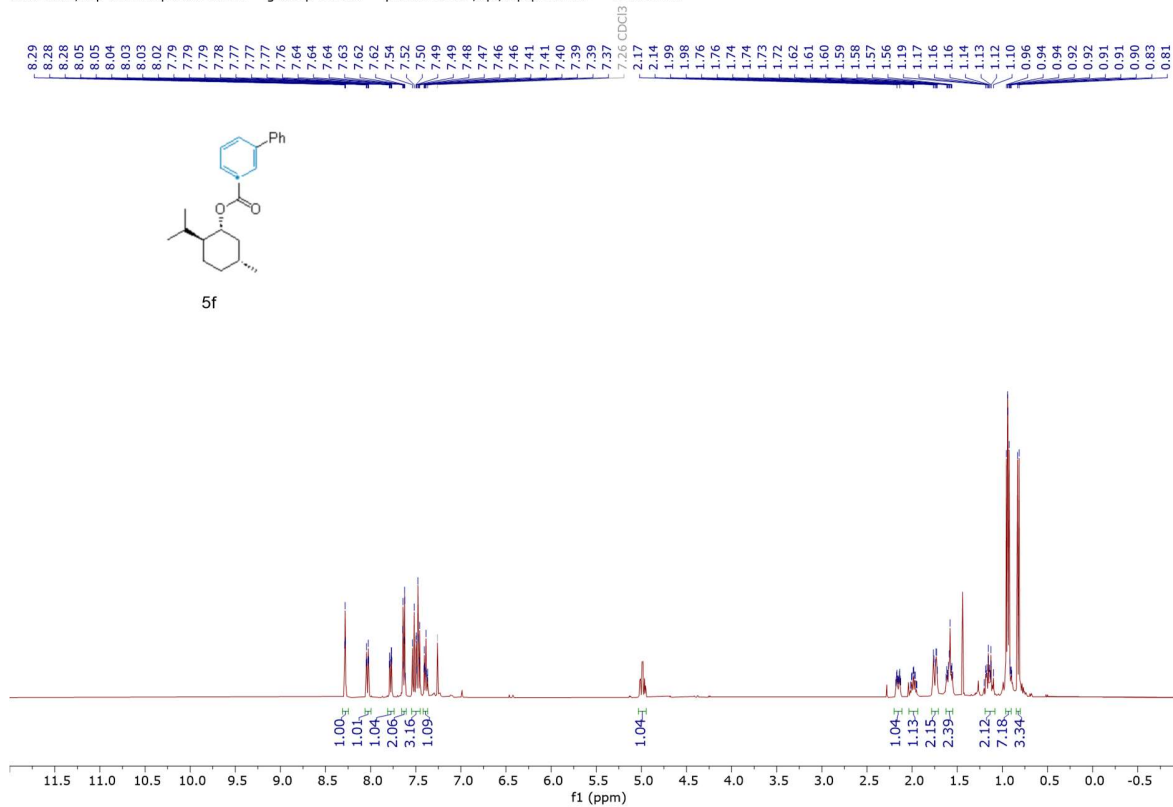
RAW Data/wfp-wb-520-carbon-CDCl3-2 — glo wfp wb 520 — carbon CDCl3 /opt/topspin av1 3 — 100.68MHz



RAW Data/wfp-wb-520-p31cpd-CDCl3-2 — glo wfp wb 520 — p31cpd CDCl3 /opt/topspin av1 3 — 162.06MHz



RAW Data/wfp-wb-528-proton-CDCl3 — glo wfp wb 528 — proton CDCl3 /opt/topspin av1 3 — 400.35MHz



RAW Data/wfp-wb-528-proton-CDCl3 — glo wfp wb 528 — proton CDCl3 /opt/topspin av1 3 — 400.35MHz

