Supporting Information

# Regioselective Palladium-Catalyzed C-H Bond Trifluoroethylation of Indoles: Exploration and Mechanistic Insight

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**Contents**

## 1. General Considerations

All commercially available compounds were used as received. Palladium catalysts, such as $Pd(OAc)_2$ and $Pd(acac)_2$, were purchased from STREM. $CF_3CH_2I$ was purchased from TCI. Norbornene was purchased from J&K. NMR spectra were recorded on a Varian Mercury-400 MHz or an Agilent-400 MHz spectrometer. ESI-MS(/MS) spectra were recorded on a Thermo TSQ (Thermo Finnigan, Quantum Access TM) triple-quadrupole mass spectrometer equipped with a standard ESI ion source. $CDCl_3$ was purchased from J&K. The chemical shifts (δ) were given in parts per million relative to internal standard TMS (0 ppm for $^1$H), $CDCl_3$ (77.0 ppm for $^{13}$C). Flash column chromatography was performed on silica gel 60 (particle size 200-300 mesh, purchased from Canada) and eluted with petroleum ether/ethyl acetate (PE/EA). DMF was directly obtained from solvent purification system of Innovation Technology Company.

## 2. Experimental Section

### 2.1 Starting Materials

Compounds **4a-4j**, **4l-4p**, **4s** and **4v** were commercial available and used as received. **4k**,[1] **4q**,[2] **4r**,[3] **4t**,[4] **4u**[4] were synthesized according to corresponding literatures.

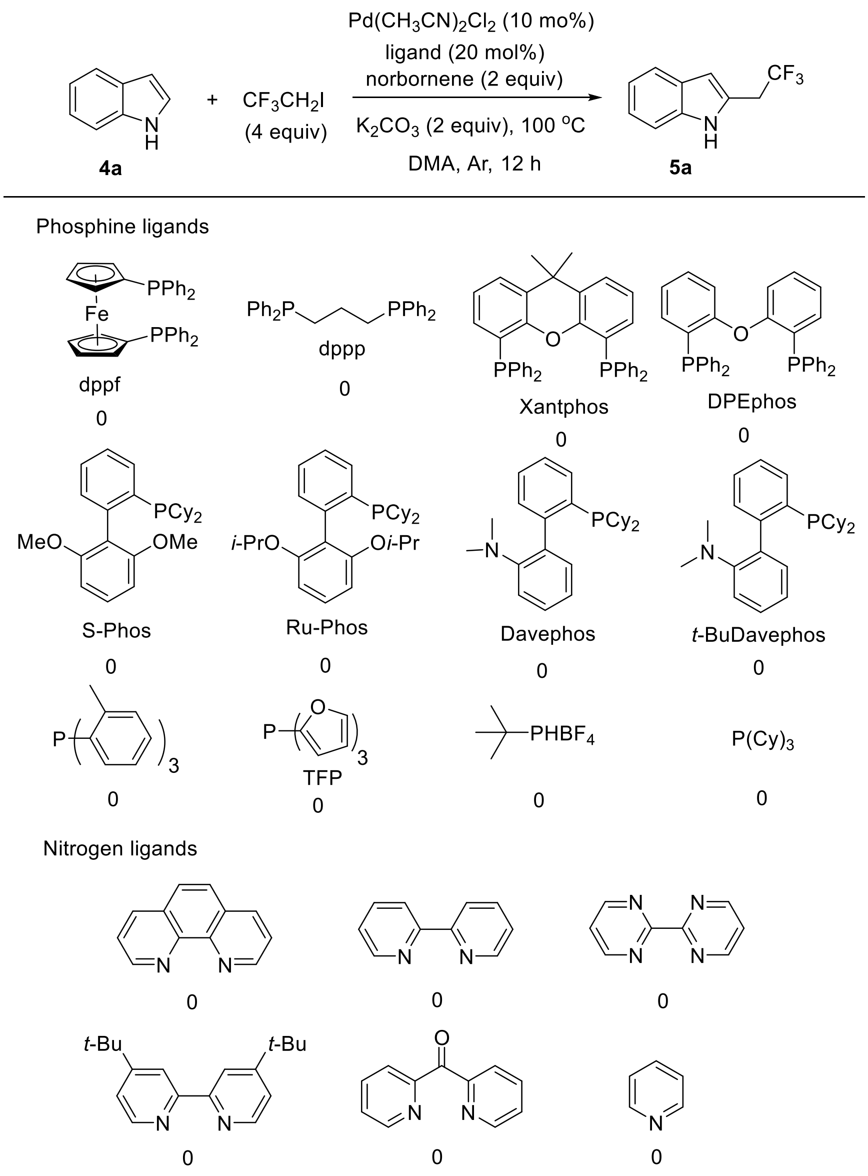
Synthesis of **4w**: To a solution of indole-3-acetic acid (1.75 g, 10 mmol) in THF (50 mL) were added DCC (1.03 g, 5 mmol) and DMAP (61 mg, 0.5 mmol), followed by cholesterol (1.93 g, 5 mmol). The reaction mixture was sirred at room temperature for 15 h, then poured into water and extracted with ethyl acetate (3×30 mL). The combined organic layers were washed with water twice and dried with anhydrous $Na_2SO_4$, filtered and concentrated under reduced pressure, the residue was purified by chromatography on silica gel with petroleum ether/ethyl acetate (5:1 to 3:1) to afford **4w** (2.06 g, 80%). $^1$H NMR (400 MHz, $CDCl_3$) δ 8.11 (br, 1H), 7.63 (d, $J$ = 8.0 Hz, 1H), 7.33 (d, $J$ = 8.0 Hz, 1H), 7.20 (td, $J$ = 7.2, 0.8 Hz, 1H), 7.16-7.12 (m, 2H), 4.36 (d, $J$ = 4.4 Hz, 1H), 4.70-4.62 (m, 1H), 3.76 (s, 2H), 2.34 (d, $J$ = 7.6 Hz, 2H), 2.04-1.79 (m, 5H), 1.64-0.98 (m, 21H), 1.02 (s, 3H), 0.92 (d, $J$ = 6.4 Hz, 3H), 0.88 (d, *J* = 6.8 Hz, 3H), 0.87 (d, *J* = 6.8 Hz, 3H), 0.68 (s, 3H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 171.6, 139.6, 136.1, 127.2, 123.0, 122.7, 122.1, 119.5, 119.0, 111.2, 108.6, 74.4, 56.7, 56.1, 49.9, 42.3, 39.7, 39.5, 38.1, 36.9, 36.6, 36.2, 35.8, 31.9, 31.8, 31.7, 28.2, 28.0, 27.8, 24.3, 23.8, 22.8, 22.6, 21.0, 19.3, 18.7, 11.8. HRMS: m/z (ESI) calculated $[M+NH_4]^+$: 561.4415, measured: 561.4413.

## 2.2 General Procedure for Palladium-Catalyzed Trifluoroethylation of Indoles.

To a dried 4 mL glass sealed tube, substrate **4** (0.2 mmol), $Pd(acac)_2$ (9.1 mg, 0.03 mmol, 15 mol %), **dbm** (17.9 mg, 0.08 mmol, 40 mol %), norbornene (37.6 mg, 0.4 mmol, 2 equiv.) and $KHCO_3$ (40.0 mg, 0.4 mmol, 2 equiv.) were added in dry DMF (1.0 mL) under Ar atmosphere. Then $CF_3CH_2I$ (120.6 mg, 0.6 mmol, 3 equiv.) was added to the solution, and the mixture was stirred at room temperature for 5 minutes. The sealed tube was subsequently immersed in a preheated oil bath at 100 $^{o}C$ for 8 hours. After that, the mixture solution was cooled to room temperature and filtered through a thin pad of silica gel. The filter cake was washed with ethyl acetate and the combined filtrate was washed with water. Then the organic layer was dried with $Na_2SO_4$ before concentration. The residue was purified by flash column chromatography to afford the product **5**. The results of **5a-5w** were listed in **Table 2-3**.

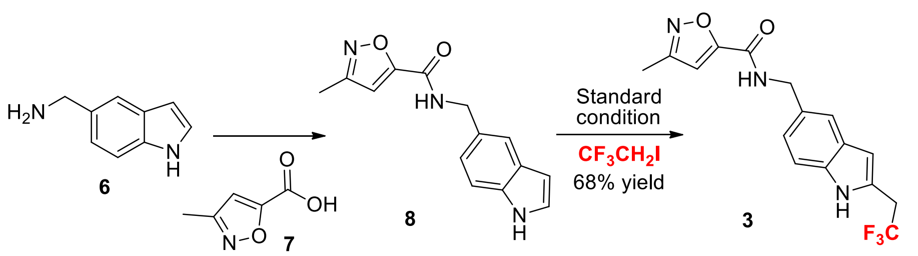
## 2.3 Ligand Screening.

**Table S1.** Phosphine and Nitrogen Ligands Screening.




[a] Reactions were run in sealed tube on 0.2 mmol with respect to indole. [b] yields are determined by $^1$H NMR and $^{19}$F NMR using N,N-Dimethyltrifluoroacetamide as an internal standard.

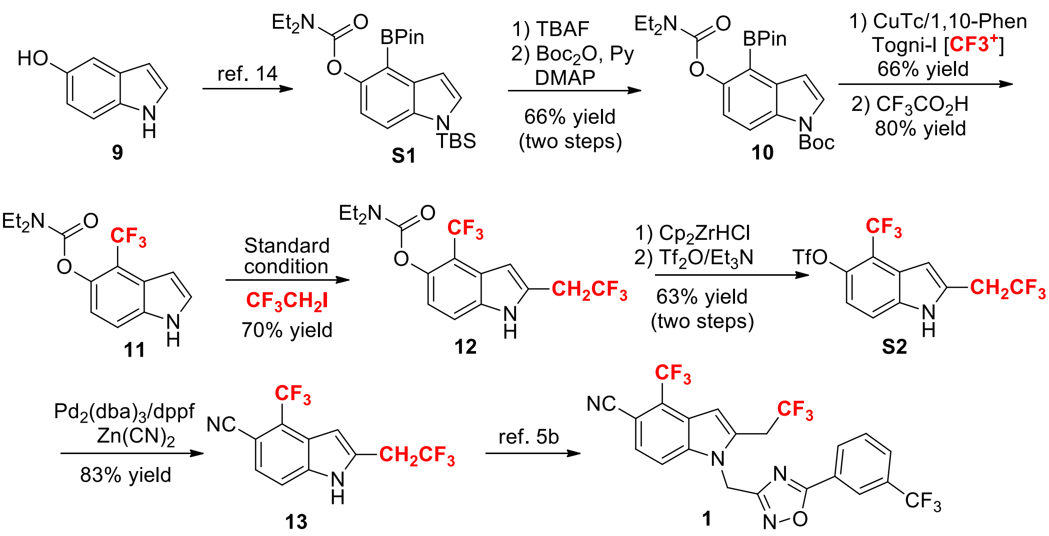
## 2.4 Synthetic Application




To a mixture of acid **7** (0.65 g, 5.13 mmol), *O*-(Benzotriazol-1-yl)-*N*,*N*,*N'*,*N'*-tetramethyluronium hexafluorophosphate (HBTU, (1.56 g, 4.10 mmol) and $Et_3N$ (1.43

mL, 10.26 mmol) in DMF (7 mL), a solution of 5-(aminomethyl)-indole **6** (0.5 g, 3.42 mmol) and $Et_3N$ (1.10 mL, 8.6 mmol) in DMF (7 mL) was added. The mixture was stirred at room temperature overnight. After that, the mixture was poured into brine, and extracted with ethyl acetate (2×30 mL). The combined organic layers were dried over anhydrous $Na_2SO_4$. The filtrate was concentrated in vacuo and the residue was purified by chromatography on silica gel with petroleum ether/ethyl acetate (5:1) to give **8** (0.68 g, 78% yield). Compound **8**: $^1$H NMR (400 MHz, $d_6$-DMSO) δ 11.06 (br, 1H), 9.41 (s, 1H), 7.49 (s, 1H), 7.37-7.33 (m, 2H), 7.08-7.07 (m, 1H), 6.95 (s, 1H), 6.40 (s, 1H), 4.52 (s, 2H), 2.29 (s, 3H). $^{13}$C NMR (100 MHz, $d_6$-DMSO) δ 163.7, 160.9, 156.0, 135.5, 129.4, 128.0, 126.1, 121.5, 119.4, 111.7, 107.4, 101.4, 43.2, 11.4. $^{19}$F NMR (376 MHz, $d_6$-DMSO) δ -63.7 (t, *J* = 10.5 Hz). HRMS: m/z (ESI) calculated $[M+H]^+$: 256.1081, measured: 256.1083.

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1 to 4:1) to afford the product **3** in 68% yield. $^1$H NMR (400 MHz, $d_6$-Acetone) δ 10.22 (br, 1H), 8.27 (br, 1H), 7.43 (s, 1H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 6.69 (s, 1H), 6.36 (s, 1H), 4.53 (d, *J* = 5.2 Hz, 2H), 3.68 (q, *J* = 10.8 Hz, 2H), 2.17 (s, 3H). $^{13}$C NMR (100 MHz, $d_6$-Acetone) δ 163.8, 160.5, 155.7, 136.2, 129.8, 128.4, 128.0, 125.7 (q, *J* = 274.9 Hz), 122.1, 119.5, 111.1, 106.8, 103.1, 43.1, 32.7 (q, *J* = 30.8 Hz), 10.3. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -64.9 (t, *J* = 10.9 Hz). HRMS: m/z (ESI) calculated $[M+H]^+$: 338.1111, measured: 338.1112.




**S1** was synthesized from commercial available 5-hydroxylindole (**9**) according to the reported procedure.[5]

Synthesis of compound **10**: To a solution of **S1** (1.30 g, 2.75 mmol) in THF (20 mL), a solution of tetrabutylammonium fluoride (TBAF, 3.4 mL, 3.4 mmol, 1 M) in THF was added dropwisely under argon atmosphere. After stirring for 30 min, the reaction mixture was quenched with water and extracted with ethyl acetate (2×30 mL). The combined organic layer was washed with water and brine, then was dried over anhydrous $Na_2SO_4$. After filtered, the filtrate was concentrated under reduced pressure to afford the crude indole product, which was dissolved in $CH_2Cl_2$ (10 mL). Then pyridine (0.30 mL, 3.58 mmol), $Boc_2O$ (0.78 g, 3.58 mmol), and DMAP (0.037 g, 0.3 mmol) were gradually added to above solution. The mixture was stirred for 24 h at room temperature. Aqueous solution of $NH_4Cl$ (10 mL) was added and the organic phase was separated. The aqueous phase was extracted with EtOAc (3×20 mL). The combined organic layers were dried over $Na_2SO_4$. The filtrate was concentrated in vacuum and the residue was purified by chromatography on silica gel with petroleum ether/ethyl acetate (8:1 to 4:1) to afford Boc protected indole **10** (0.83 g, 66% yield). $^1$H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, $J$ = 6.8 Hz, 1H), 7.59 (s, 1H), 7.08 (d, $J$ = 3.2 Hz, 1H), 7.21 (d, $J$ = 8.8 Hz, 1H), 3.53-3.38 (m, 4H), 1.65 (s, 9H), 1.34 (s, 12H), 1.34-1.18 (m, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 155.2, 152.5, 149.6, 136.3, 132.2, 126.5, 118.7, 118.1, 118.1, 109.4, 83.5, 83.2, 41.8, 41.5, 28.1, 24.9, 14.0, 13.4. HRMS:

m/z (ESI) calculated $[M+H]^+$: 459.2661, measured: 459.2667.

Synthesis of compound **11**: CuTc (19 mg, 0.1 mmol), 1,10-phenanthroline (36 mg, 0.20 mmol), $LiOH.H_2O$ (83 mg, 2.0 mmol), indole **10** (229 mg, 0.5 mmol) and Togni's reagent (248 mg, 0.75 mmol) were placed into an oven-dried sealed tube equipped with a stirring bar under Ar. Freshly distilled $CH_2Cl_2$ (4.0 mL) was added. The reaction mixture was stirred at 45 $^oC$ for 12 h. After cooling to room temperature, the mixture was washed by brine (10 mL) and the aqueous phase was extracted with $CH_2Cl_2$ (3 × 10 mL). The combined organic extracts were dried over anhydrous $Na_2SO_4$. The filtrate was concentrated in vacuum and the residue was purified by chromatography on silica gel with petroleum ether/ethyl acetate (15:1 to 8:1) to afford trifluoromethylated indole (132 mg, 66% yield), which was dissolved in dichloromethane (10 mL). To a cooled solution, trifluoroacidic acid (2 mL) was added and the mixture was stirred for 30 min at 0 ℃. After 3 h, saturated $NaHCO_3$ aq was added slowly. The mixture was extracted with ethyl acetate (3×20 mL). The combined organic layers were dried with anhydrous $Na_2SO_4$, and the filtrate was concentrated under reduced pressure. The residue was purified by chromatography on silica gel with petroleum ether/ethyl acetate (4:1) to give indole **11** (80 mg, 80% yield). $^1H$ NMR (400 MHz, $CDCl_3$) δ 9.06 (br, 1H), 7.05 (d, *J* = 8.8 Hz, 1H), 7.01-6.99 (m, 1H), 6.81 (d, *J* = 8.8 Hz, 1H), 6.50 (s, 1H), 3.51 (q, *J* = 6.8 Hz, 2H), 3.43 (q, *J* = 6.8 Hz, 2H), 1.29 (t, *J* = 6.8 Hz, 3H), 1.24 (t, *J* = 6.8 Hz, 3H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 155.1, 142.6, 133.9, 127.3, 124.7 (q, *J* = 272.0 Hz), 124.4, 117.2, 115.4, 112.9 (q, *J* = 31.1 Hz), 101.5, 42.2, 41.8, 13.8, 13.2. $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -57.0 (s). HRMS: m/z (ESI) calculated $[M+H]^+$: 301.1396, measured: 301.1403.

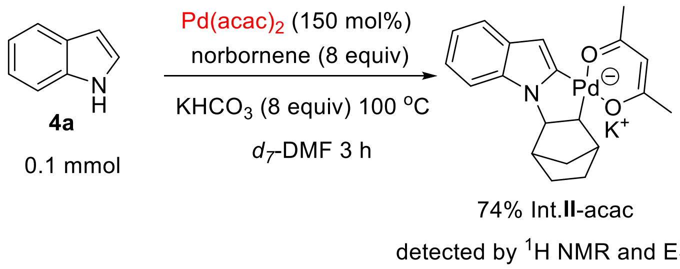
Synthesis of compound **12**: The trifluoroethylation of indole **11** was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1 to 4:1) to afford the product **12** (54 mg, 70% yield). $^1H$ NMR (400 MHz, $CDCl_3$) δ 9.03 (br, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 6.80 (d, *J* = 8.8 Hz, 1H), 6.49 (s, 1H), 3.51 (q, *J* = 7.2 Hz, 2H), 3.47 (q, *J* = 10.8 Hz, 2H), 3.43 (q, *J* = 7.2 Hz, 2H), 1.29 (t, *J* = 7.2 Hz, 3H), 1.24 (t, *J* = 7.2 Hz, 3H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 155.0, 142.8 (q, *J* = 3.3 Hz), 134.5, 130.1, 124.9 (q, $J$ = 276.8 Hz), 124.7 (q, $J$ = 271.9 Hz), 124.6, 117.6, 115.4, 112.7 (q, $J$ = 30.9 Hz), 102.6 (q, $J$ = 3.6 Hz), 42.3, 41.9, 33.2 (q, $J$ = 31.3 Hz), 13.8, 13.1. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -57.0 (s), -65.5 (t, $J$ = 10.5 Hz). HRMS: m/z (ESI) calculated $[M+H]^+$: 383.1189, measured: 383.1190.

Synthesis of compound **S2**: To a suspension of $Cp_2Zr(H)Cl$ (129 mg, 0.5 mmol) in THF (0.5 mL), a solution of **12** (38 mg, 0.1 mmol) in THF (0.5 mL) was added at room temperature. The resulting mixture was stirred at room temperature for overnight. The reaction mixture was quenched with 1 N HCl (0.3 mL), and then neutralized with saturated $NaHCO_3$ aq. The mixture was extracted with EtOAc (3×20 mL). The combined organic layer was dried over anhydrous $Na_2SO_4$, and the filtrate was concentrated under reduced pressure to give a crude phenol (21 mg, 74% yield) which was dissolved in dry dichloromethane (1 mL) under Ar. To a cooled solution, $Et_3N$ (30 μL, 0.20 mmol) and $Tf_2O$ (16 μL, 0.10 mmol) were added gradually at 0 $^{o}$C. The reaction mixture was warmed up to room temperature and stirred for 5 h. The reaction was quenched with water and extracted with ethyl acetate (3×10 mL). The combined organic layers were dried over anhydrous $Na_2SO_4$, and the filtrate was concentrated under reduced pressure. The residue was purified by chromatography on silica gel with petroleum ether/ethyl acetate (4:1) to give triflate ester **S2** (26 mg, 63% yield for two steps). $^1$H NMR (400 MHz, $d_6$-Acetone) δ 11.35 (br, 1H), 7.90 (d, $J$ = 9.2 Hz, 1H), 7.35 (d, $J$ = 8.8 Hz, 1H), 6.84 (s, 1H), 4.00 (q, $J$ = 10.8 Hz, 2H). $^{13}$C NMR (100 MHz, $d_6$-Acetone) δ 139.0 (q, $J$ = 3.3 Hz), 136.2, 135.5, 125.3 (q, $J$ = 274.2 Hz), 125.2, 123.7 (q, $J$ = 271.7 Hz), 118.5 (q, $J$ = 317.7 Hz), 116.6, 115.4, 112.5 (q, $J$ = 31.4 Hz), 102.9 (q, $J$ = 3.6 Hz), 32.5 (q, $J$ = 31.0 Hz). $^{19}$F NMR (376 MHz, $d_6$-Acetone) δ -51.5 (s), -60.7 (t, $J$ = 10.5 Hz), -69.5 (d, $J$ = 1.5 Hz). HRMS: m/z (ESI) calculated $[M+H]^+$: 415.997, measured: 416.000.

Synthesis of compound **13**: To a solution $Pd_2(dba)_3$ (6.4 mg, 0.007 mmol%) and dppf (7.7 mg, 0.014 mmol) in mixture solvent of NMP and $H_2O$ (0.5 mL, 8:1), a solution of **S2** (26 mg, 0.068 mmol) in NMP/$H_2O$ (0.5 mL) was added under Ar. The mixture was stirred at room temperature for 15 min, then $Zn(CN)_2$ (8 mg, 0.068 mmol) was added under Ar. The reaction mixture was gradually heated to 80 $^{o}$C for 3 h. After cooling to room temperature, the mixture was concentrated under reduced pressure, the residue was purified by chromatography on silica gel with petroleum ether/ethyl acetate (4:1 to 2:1) to give cynation product **13** (16 mg, 83% yield). $^{1}$H NMR (400 MHz, $d_6$-DMSO) δ 12.38 (br, 1H), 7.86 (d, $J$ = 8.8 Hz, 1H), 7.71 (d, $J$ = 8.0 Hz, 1H), 6.73 (s, 1H), 4.00 (q, $J$ = 10.8 Hz, 2H). $^{13}$C NMR (100 MHz, $d_6$-DMSO) δ 139.4, 134.5, 126.8, 125.8 (q, $J$ = 275.1 Hz), 124.7 (q, $J$ = 2.8 Hz), 124.2 (q, $J$ = 272.9 Hz), 122.7 (q, $J$ = 32.1 Hz), 117.8, 116.5, 102.5, 99.9 (q, $J$ = 3.1 Hz), 32.5 (q, $J$ = 30.4 Hz). $^{19}$F NMR (376 MHz, $d_6$-DMSO) δ -52.0 (s), -58.9 (t, $J$ = 10.9 Hz). HRMS: m/z (EI) calculated $[M]^+$: 292.0435, measured: 292.0437.

## 3. Mechanism Studies

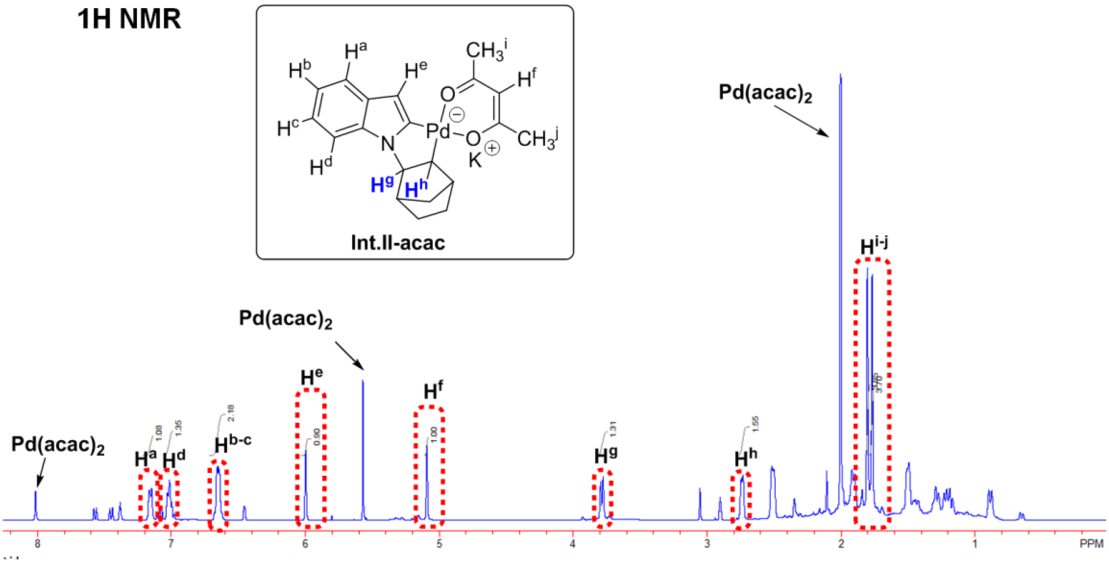
### 3.1 Characterization of anionic palladacycle



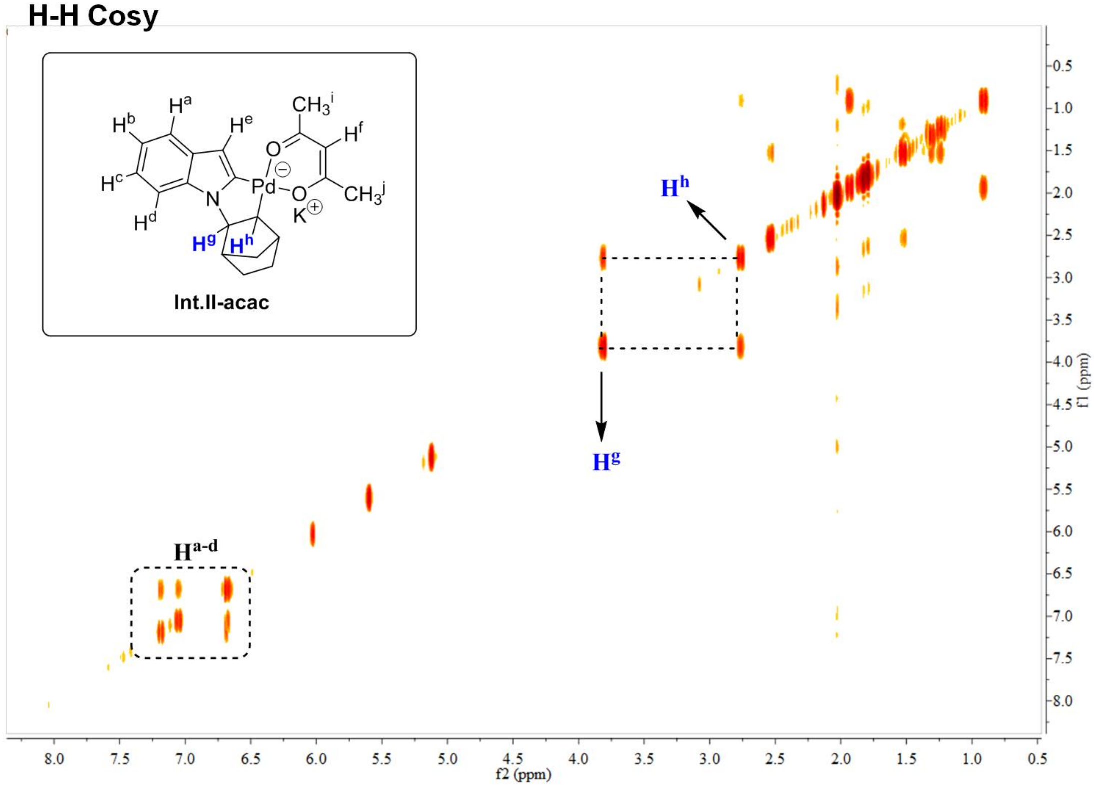

(S1)

To a dried 4 mL glass sealed tube, substrate **4a** (11.7 mg, 0.1 mmol), $Pd(acac)_2$ (45.5 mg, 0.15 mmol, 150 mol %), norbornene (75.2 mg, 0.8 mmol, 8 equiv) and $KHCO_3$ (80.0 mg, 0.8 mmol, 8 equiv) were dissolved in $d_7$-DMF (1 mL) under Ar atmosphere. The sealed tube was subsequently immersed in a preheated oil bath at 100 °C for 3 hours. After that, the reaction was cooled to room temperature, then most of norborene was removed under vacuum and the mixture was filtered through PTFE Syringe Filter to give a clear solution. The solution was analyzed by $^{1}$H NMR using $CH_2Br_2$ as an internal standard and ESI-MS to observe the **Int.II-acac**. The spectra of $^{1}$H NMR, COSY, NOESY and ESI-MS were listed in below. Unfortunately, we were failed to get pure palladacycle complex **int.II-acac**.

## 1H NMR




## H-H Cosy



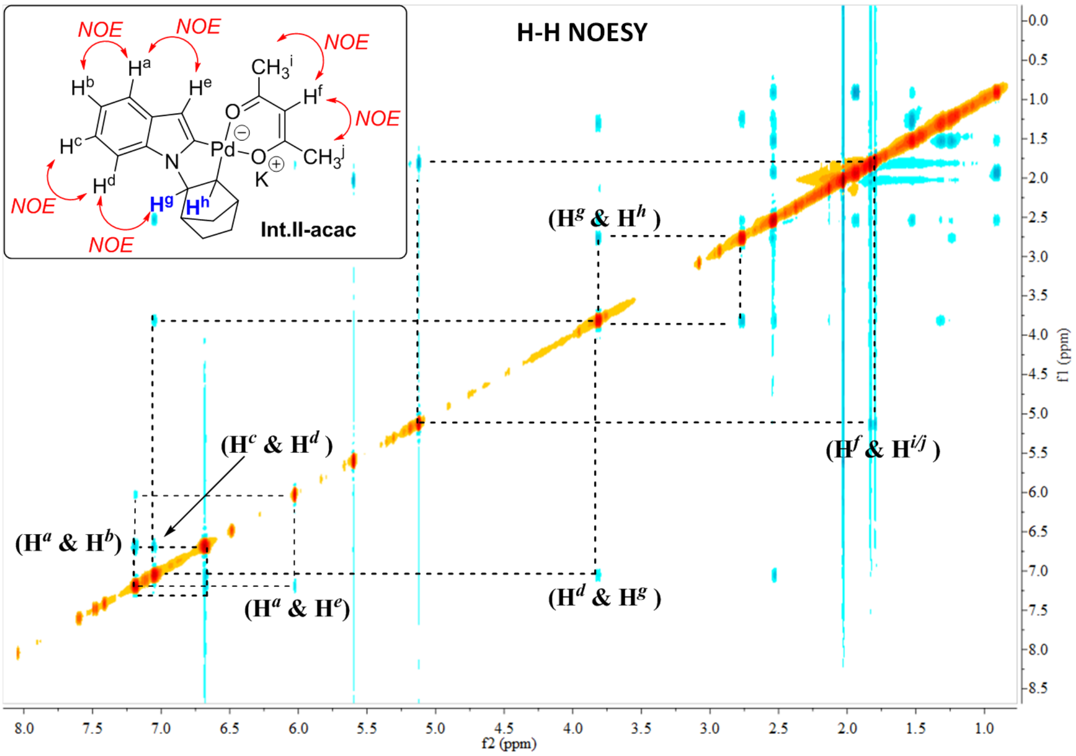



**Figure S1.** Crude [1]H NMR, COSY and NOSEY Spectra of Reaction in $d_7$-DMF [containing extra Pd(acac)$_2$].

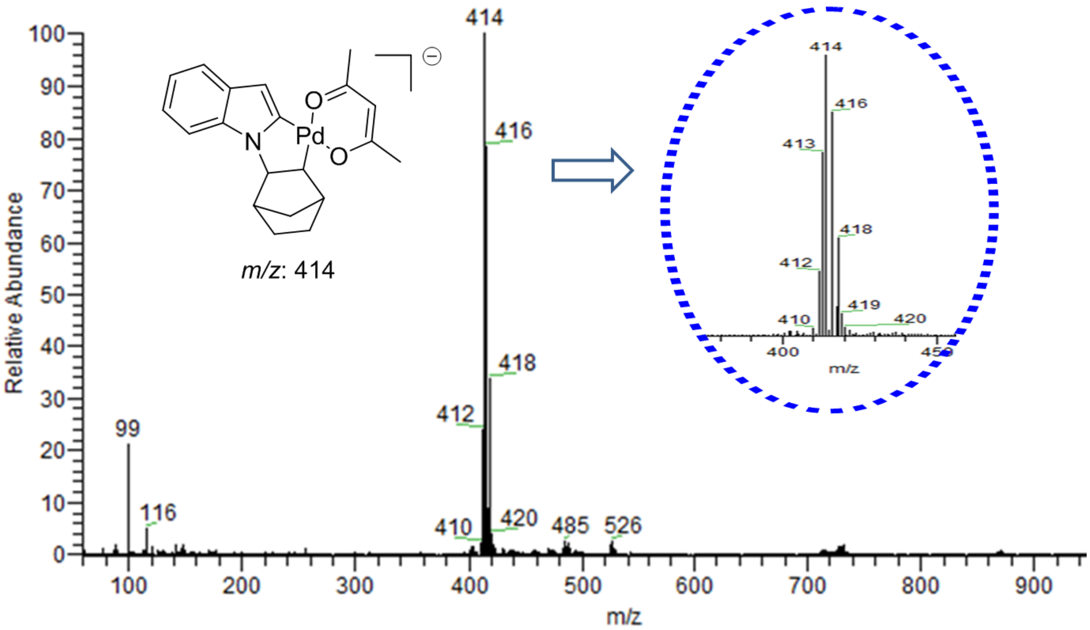
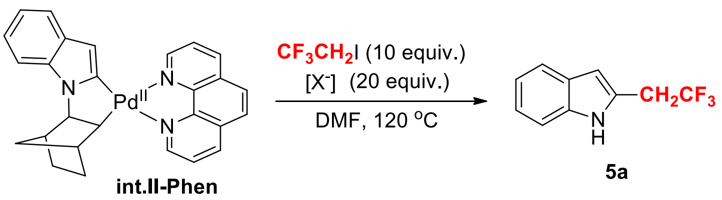



**Figure S2.** The negative ion mode ESI-MS spectrum for the diluted reaction solution containing palladacycle complex **int-II-acac**.

## 3.2. Stoichiometric Reaction

### The trifluoroethylation reaction of int.II-Phen



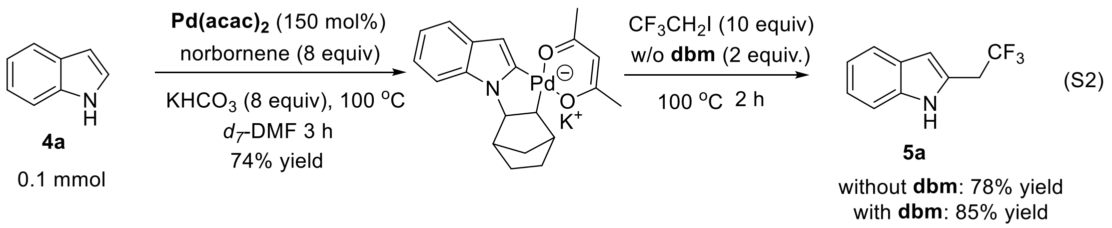

| [X$^-$] | -- | LiCl | KOAc | NaOPh | $KO_2CCF_3$ | Kacac•1/$_2H_2O$ |
|---|---|---|---|---|---|---|
| **5a** Yield | 0 | 0 | 0 | 0 | 0 | 10% (15%)[a] |

[a] Kacac •1/$_2H_2O$ (50 equiv.) was used.

Complex **int. II-Phen** was prepared according to Bach's procedure.[6]

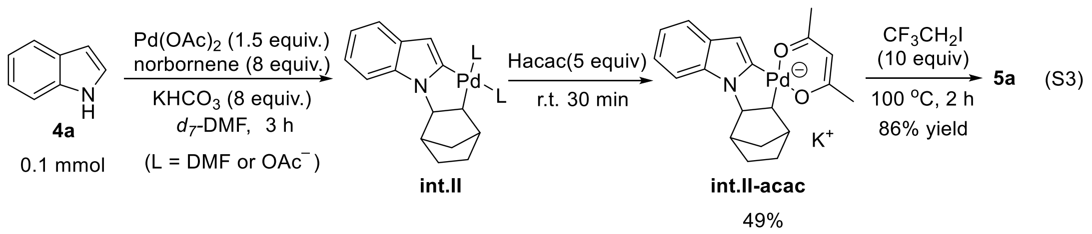
To a 4 mL sealed tube was weight into **int. II-Phen** (12.4 mg, 0.025 mmol) and MX (0.5 mmol, 20 equiv), then the mixture was dissolved with DMF (1.0 mL) under $N_2$. After quickly addition of $CF_3CH_2I$ (52.5 mg, 0.25 mmol, 10 equiv), the tube was sealed and subsequently immersed in a preheated oil bath at 120 $^oC$ for 6 hours. After that, the mixture solution was cooled to room temperature and was filtered through a thin pad of celite. The filter was analyzed by $^{19}F$ NMR with $CF_3$-DMA as internal standard. Results were listed above. No desired product **5a** was observed in the absence or presence of LiCl, KOAc, NaOPh and $KO_2CCF_3$. However, the reaction provided product **5a** in 10% yield in the presence of Kacac, and the yield was further increased to 15% by increasing Kacac loading to 50 equivalent.

**With Pd(acac)$_2$** (path b):



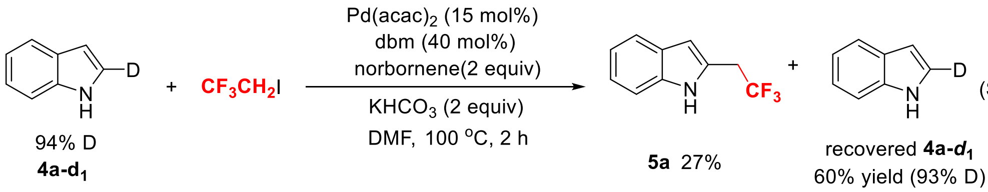

For above cooled mixture solution in **3.1**, $CF_3CH_2I$ (148.7 mg, 0.74 mmol, 10 equiv) and **dbm** (0 or 2 equiv.) were added, and the mixture was sealed in a 4 mL sealed tube, which was subsequently immersed in a preheated oil bath at 100 $^oC$ for 2 hours. After that, the mixture solution was cooled to room temperature and was filtered through a thin pad of silica gel. The filter cake was washed with ethyl acetate and the combined filtrate was washed with water. Then the organic layer was dried with $Na_2SO_4$ before concentration. The residue was analyzed by $^1H$ NMR with $CF_3$-DMA as internal standard. The reaction provided the desired product **5a** in 78% yield in the absence of **dbm**, and 85% yield with **dbm** (eq S2).

**With $Pd(OAc)_2$ and H-acac (path a):**




To a dried 4 mL glass sealed tube, substrate **4a** (11.7 mg, 0.1 mmol), $Pd(OAc)_2$ (33.7 mg, 0.15 mmol, 1.5 equiv), norbornene (75.2 mg, 0.8 mmol, 8 equiv) and $KHCO_3$ (80.0 mg, 0.8 mmol, 8 equiv) were added in $d_7$-DMF (0.5 mL) under Ar atmosphere. Then the mixture was stirred at room temperature for 5 minutes and the sealed tube was subsequently immersed in a preheated oil bath at 100 $^oC$ for 3 hours. After that, the reaction was cooled to room temperature and H-acac (50 mg, 0.5 mmol) was added to stir for 30 minutes. Then $CH_2Br_2$ was added as an internal standard to determine the yield of **int.II-acac** by crude $^1H$ NMR (49% yield). After monitored by NMR, the mixture was filtered through PTFE Syringe Filter to remove the insoluble substance and vacuumed to remove most norbornene. Additional DMF (0.5 mL) and $CF_3CH_2I$ (98.5 mg, 0.49 mmol, 10 equiv) were added to the residue. The sealed tube was subsequently immersed again in a preheated oil bath at 100 $^oC$ for 2 hours. Then the reaction was cooled to room temperature with the work up procedure as above. The residue was analyzed by $^1H$ NMR with $CF_3$-DMA as internal standard to give **5a** in 86% yield. It is mentioned that, however, the reaction provided trace amount of **5a** in the absence of H-acac.

### 3.3 Deuterium Labeling Experiments

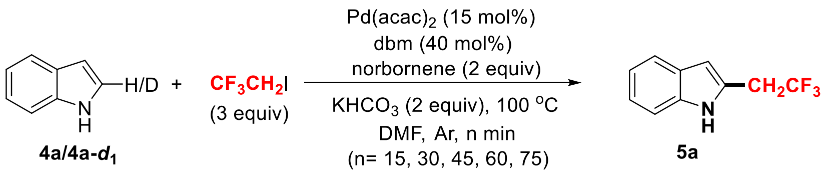



(S4)

With the literature procedure, deuterium-labeled **4a-*d*$_1$**[7] was synthesized in 94% deuterium incorporation. To a dried 4 mL glass sealed tube, **4a-*d*$_1$** (23.6 mg, 0.2 mmol), Pd(acac)$_2$ (9.1 mg, 0.03 mmol, 15 mol %), **dbm** (17.9 mg, 0.08 mmol, 40 mol %), norbornene (37.6 mg, 0.4 mmol, 2 equiv) and $KHCO_3$ (40.0 mg, 0.4 mmol, 2 equiv) were added in dry DMF (1.0 mL) under Ar atmosphere. Then $CF_3CH_2I$ (120.6 mg, 0.6 mmol, 3 equiv) was added and the mixture was stirred at room temperature for 5 minutes. The sealed tube was subsequently immersed in a preheated oil bath at 100 °C for 2 hours. After that, the reaction was cooled to room temperature and the mixture was filtered through a thin pad of silica gel. The filter cake was washed with ethyl acetate and the combined filtrate was washed with water. Then the organic layer was dried with $Na_2SO_4$ before concentration. The residue was purified by flash column chromatography using PE:EA=20:1 to give **5a** in 27% yield, and **4a-*d*$_1$** was recovered in 60% yield with 93% D.

### 3.4 Kinetic Isotopic Effect.

### 3.4.1 Kinetic Isotope Effect of 2-C-H bond of Indole




(S5)

The initial rate of the reaction was determined by measurement of five parallel individual experiment yields after running for 15 minutes, 30 minutes, 45minutes, 60 minutes and 75 minutes respectively: To a dried 4 mL glass sealed tube, substrate **4a** (0.2 mmol, 23.4 mg) or **4a-*d*$_1$** (0.2 mmol, 23.6 mg), Pd(acac)$_2$ (9.1 mg, 0.03 mmol, 15 mol %), dbm (17.9 mg, 0.08 mmol, 40 mol %), norbornene (37.6 mg, 0.4 mmol, 2 equiv) and $KHCO_3$ (40.0 mg, 0.4 mmol, 2 equiv) were dissolved in dry DMF (1.0 mL) under Ar atmosphere. Then $CF_3CH_2I$ (120.6 mg, 0.6 mmol, 3 equiv) was added and the mixture was stirred at room temperature for 5 minutes. The sealed tube was subsequently immersed in a preheated oil bath at 100 °C for 15minutes. After that, the reaction was immersed in an ice-water bath immediately to cool the mixture and then the mixture was filtered through a thin pad of silica gel. The filter cake was washed with ethyl acetate and the combined filtrate was concentrated. The residue was analyzed by $^{19}F$ NMR with $CF_3$-DMA as internal standard. The results were shown in below.

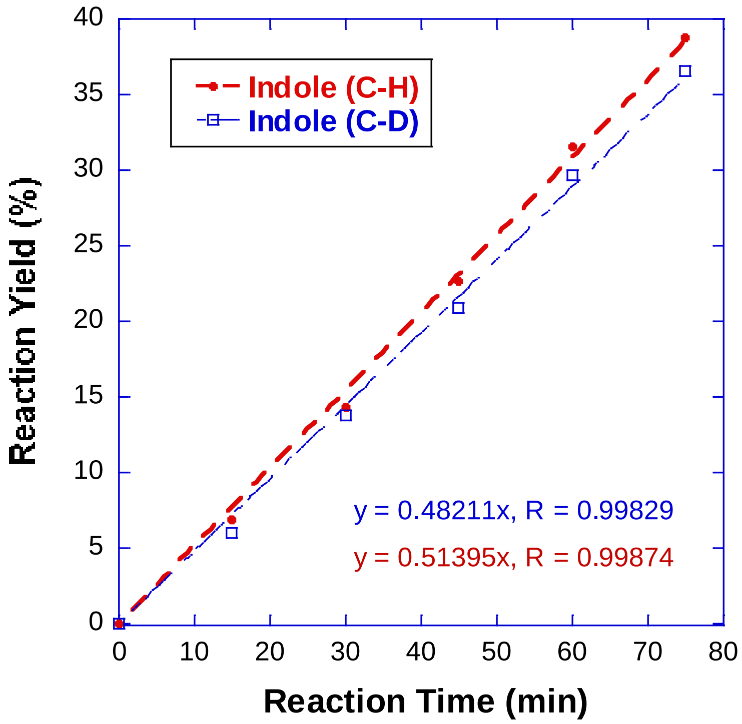
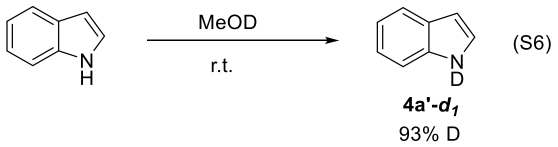



**Figure S3.** The initial rate of indole (C-H) and 2-D-indole (C-D) in standard condition. KIE(C-H) = $k_H/k_D$ = 0.514/0.482 = 1.1

**3.4.2 Kinetic Isotope Effect Study of N-H bond of indole.**

**Synthesis of 4a'-*d₁*:**




N-deuterium labeled indole **4a'-*d*$_1$** was synthesized as following procedure: In a dried 10 mL schlenk tube, indole (1.0 g, 8.55 mmol) was dissolved in MeOD (6 mL, 230 mmol) and the mixture was stirred in room temperature for 4 hours. Then the mixture was concentrated under vacuum to remove the solvent. MeOD (6 mL) was added into the schlenk tube again and the mixture was stirred in room temperature for another 4 hours. After that, the mixture was concentrated under vacuum to give quantitative yield of the product **4a'-*d*$_1$** with 93% D.

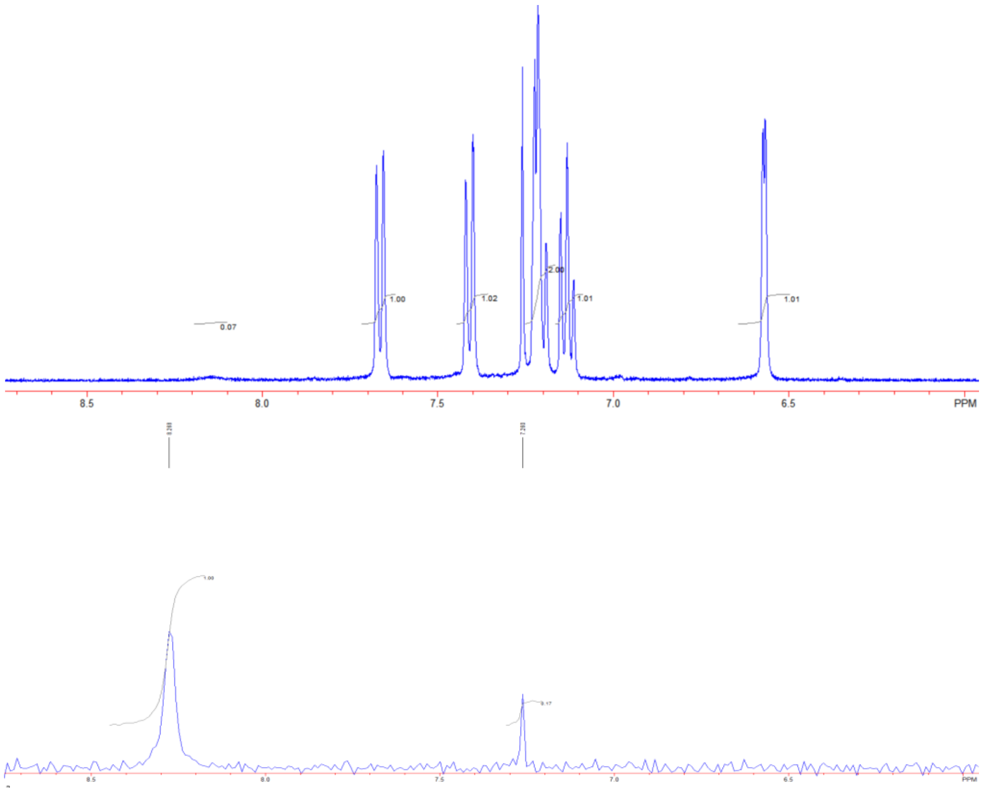
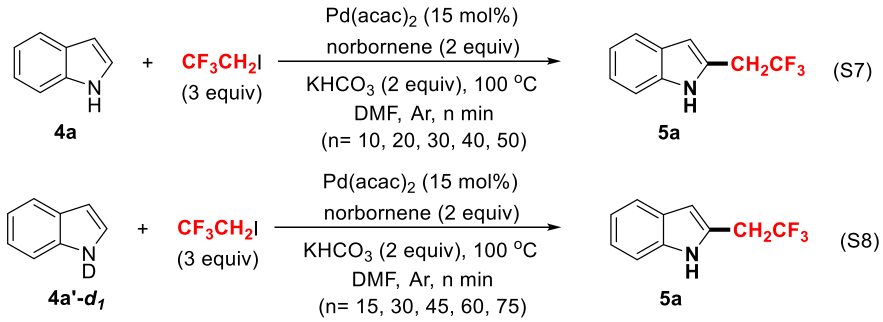


**Figure S4.** $^1$H NMR of **4a'-*d*$_1$** in $CDCl_3$ (top) and $^2$H NMR (bottom) in $CHCl_3$**.**

**Measurement of KIE:**

The initial rate of the reaction was determined by measurement of five parallel individual experiments yield. *Notes*: $KHCO_3$ and **dbm** were added into the MeOD (6 mL) and the mixture was stirred for 4 hours in 60 °C. Then the solvent was removed and the procedure was repeated for twice to make sure the hydrogen of $KHCO_3$ and

**dbm** could be replaced by deuterium if the H/D exchanged could happen in the system.




To a dried 4 mL glass sealed tube, substrate **4a'-*d₁*** (0.2 mmol, 23.6 mg), $Pd(acac)_2$ (9.1 mg, 0.03 mmol, 15 mol %), norbornene (37.6 mg, 0.4 mmol, 2 equiv) and pretreated $KHCO_3$ (40.0 mg, 0.4 mmol, 2 equiv) were added in dry DMF (1.0 mL) under Ar atmosphere. Then $CF_3CH_2I$ (120.6 mg, 0.6 mmol, 3 equiv) was added and the mixture was stirred at room temperature for 5 minutes. The sealed tube was subsequently immersed in a preheated oil bath at 100 $^{o}C$ for 15 minutes or defined time. After that, the reaction was immersed in an ice-water bath immediately and then the mixture was filtered through a thin pad of celite. The filter cake was washed with ethyl acetateand the combined filtrate was concentrated. The residue was analysed by $^{19}F$ NMR with $CF_3$-DMA as internal standard.

For the results of indole (N-H), the results were obtained with the same procedure as above with non-deuterium substrate and reagents. The KIE values were measured in the left of Figure S5. Furthermore, the reactions were also conducted in the presence of dbm (40 mol%) with the same procedure, and the results were listed in the right of Figure S5.

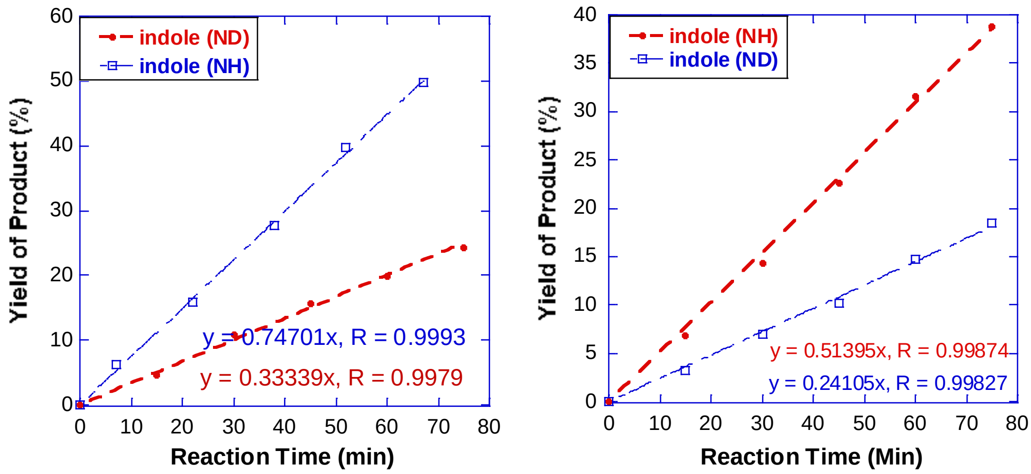



**Figure S5.** The initial rate of **4a** and **4a'-*d*₁** in standard condition: **Left**, without **dbm**, KIE(N-H) = $k_H/k_D$ = 0.7415/0.3237 = 2.3; **Right**, with **dbm**, KIE = $k_H/k_D$ = 2.1.

## 3.5 Kinetic Studies

**General Information:**

The reaction between indole **4a** and $CF_3CH_2I$ under standard conditions was selected as the model reaction for kinetic studies. The kinetic of the 2-trifluoroethylation reaction was monitored by measurement of five parallel individual experiments with different reaction time, in which the conversation is the range of 0 ~ 20% and all the five reactions were conducted in the same preheated oil bath. The kinetic measurements were conducted by using different concentrations of each component. The procedure was the same as above in section 3.4.

### 3.5.1 Dependence of Initial-Rate on [$CF_3CH_2I$]

The plot showed that the initial rate has a zero-order dependence on [$CF_3CH_2I$] (Figure S6).

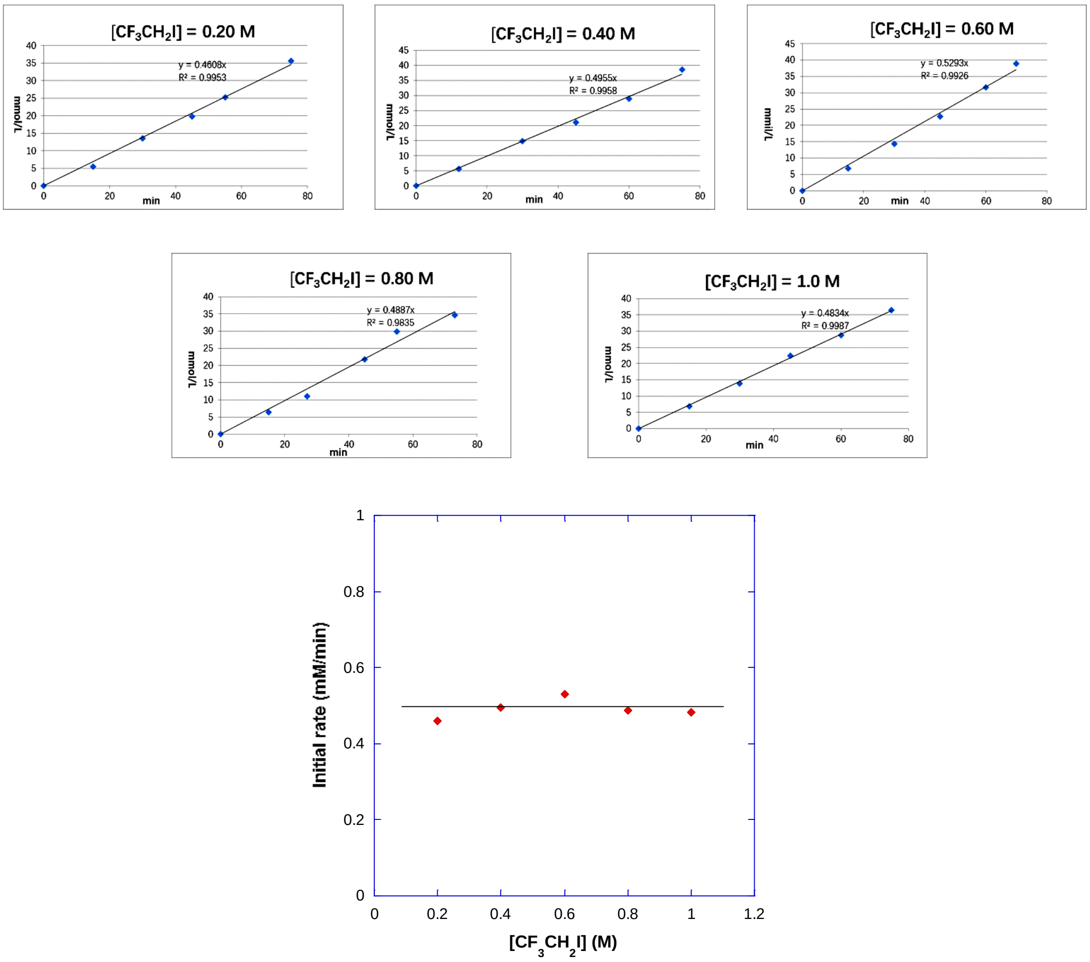



**Figure S6.** Kinetic Data: Initial Rate Dependence on [$CF_3CH_2I$]: [$CF_3CH_2I$] = 0.20-1.00 M, [Pd(acac)$_2$] = 0.03 M, [norbornene] = 0.40 M, [indole] = 0.20 M, [dbm] = 0.08 M, [$KHCO_3$] = 0.40 M in DMF, 100 $^{o}$C.

### 3.5.2 Dependence of Initial-Rate on [Norbornene]

The plot showed that the initial rate has a zero-order dependence on [Norbornene] (Figure S7).

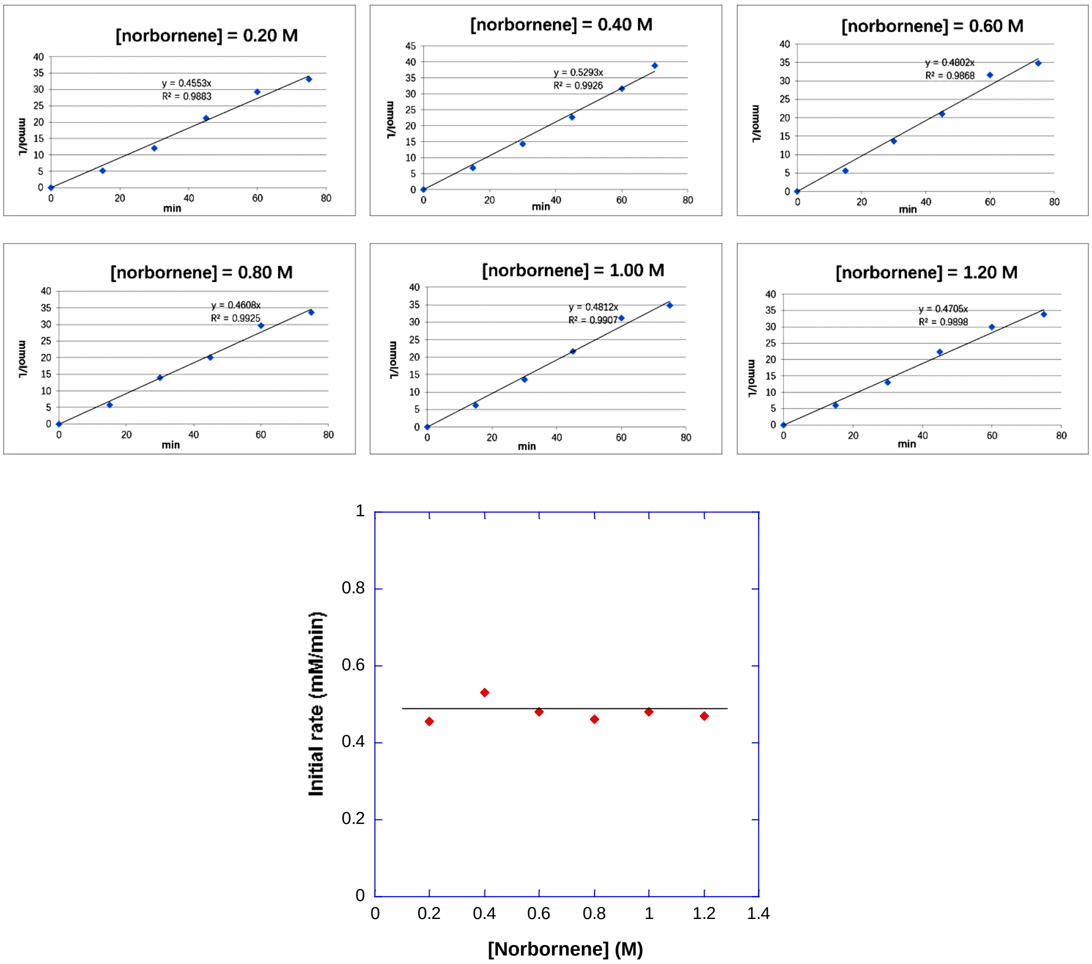



**Figure S7.** Kinetic Data: Initial Rate Dependence on [norbornene]: [norbornene] = 0.20-1.20 M, [Pd(acac)$_2$] = 0.03 M, [$CF_3CH_2I$] = 0.60 M, [indole] = 0.20 M, [dbm] = 0.08 M, [$KHCO_3$] = 0.40 M in DMF, 100 $^{o}$C.

### 3.5.3 Dependence of Initial-Rate on [Pd(acac)$_2$]

The plot showed that the initial rate has a first-order dependence on [Pd(acac)$_2$] (Figure S8).

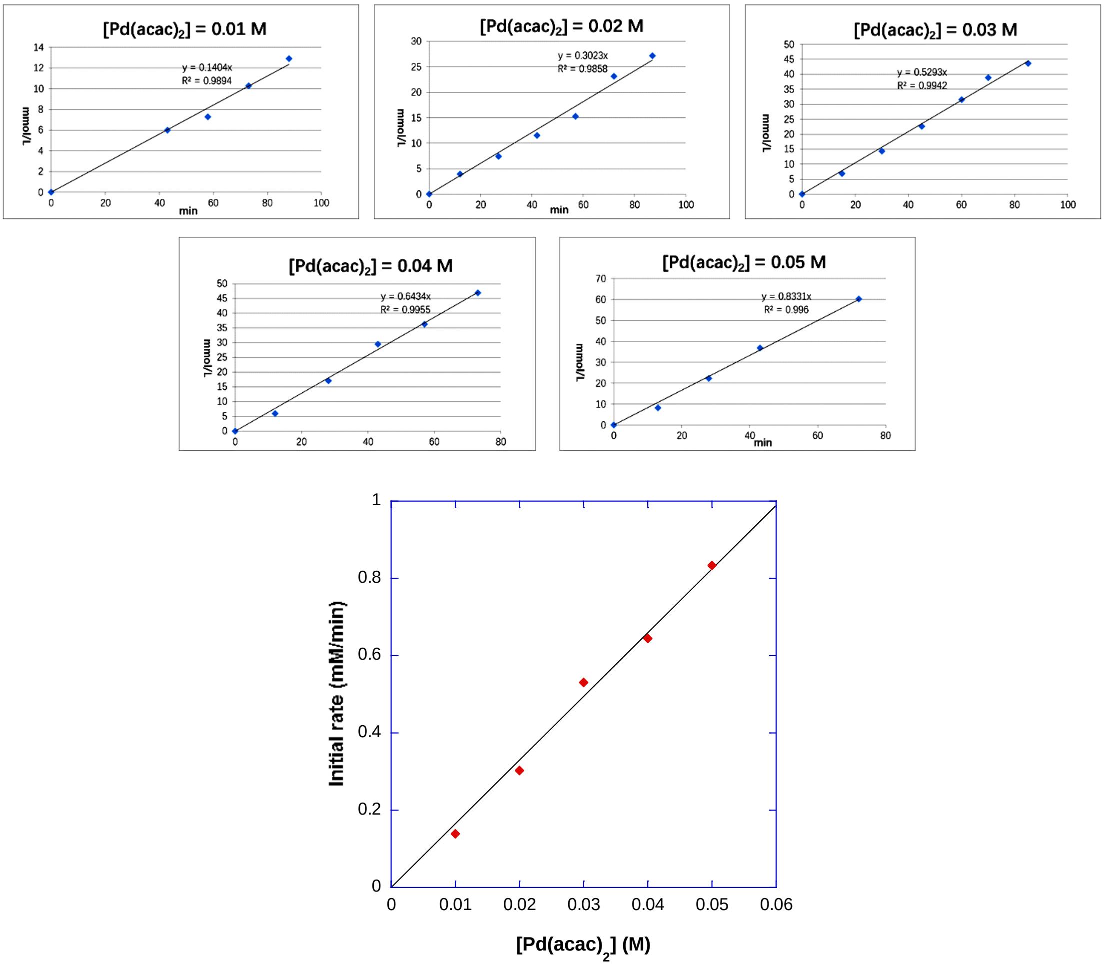



**Figure S8.** Kinetic Data: Initial Rate Dependence on [Pd(acac)$_2$]: [Pd(acac)$_2$] = 0.01-0.05 M, [norbornene] = 0.40 M, [$CF_3CH_2I$] = 0.60 M, [indole] = 0.20 M, [dbm] = 0.08 M, [$KHCO_3$] = 0.40 M in DMF, 100 $^{o}$C.

### 3.5.4 Dependence of Initial-Rate on [Indole]

The plot showed that the initial rate has saturation dependence on [indole] (Figure S9).

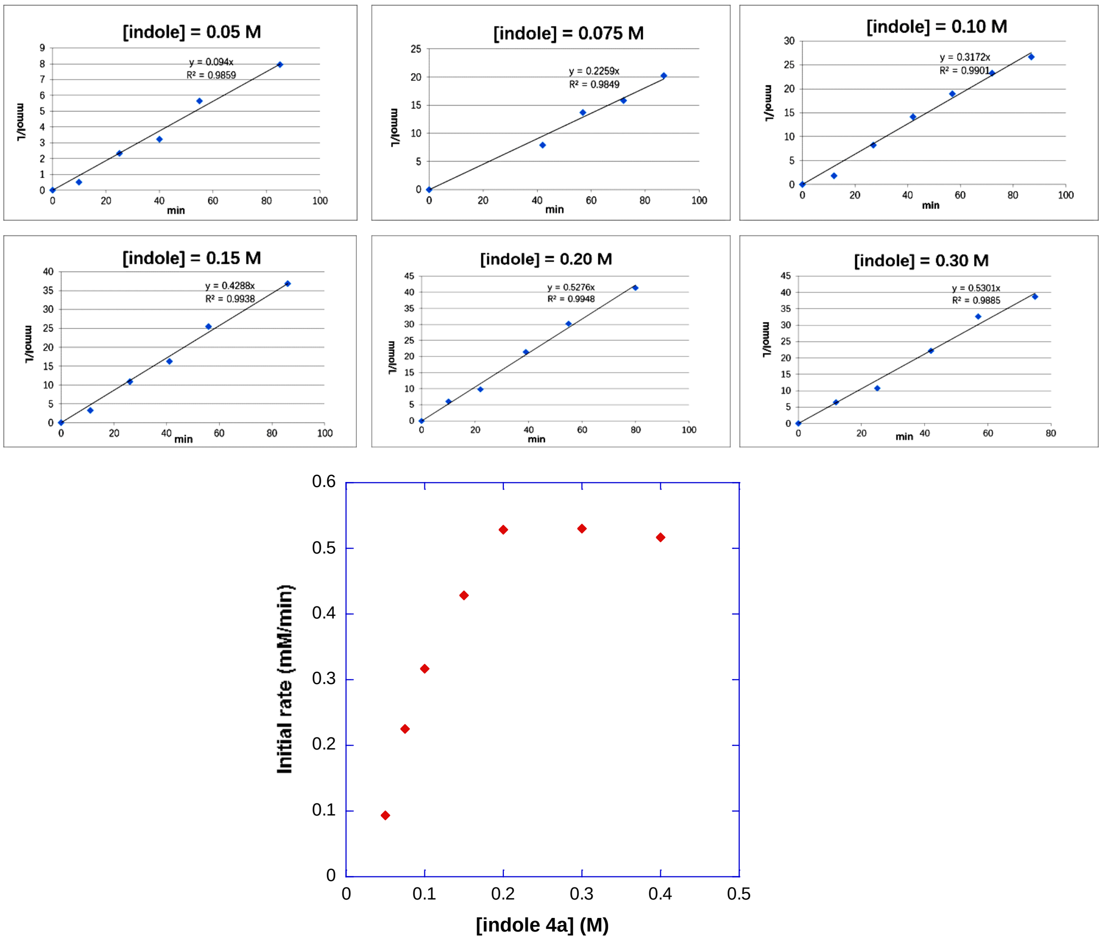



**Figure S9.** Kinetic Data: Initial Rate Dependence on [indole]: [indole] = 0.05-0.40 M, [Pd(acac)$_2$] = 0.03 M, [norbornene] = 0.40 M, [$CF_3CH_2I$] = 0.60 M, [dbm] = 0.08 M, [$KHCO_3$] = 0.40 M in DMF, 100 $^{o}$C.

### 3.5.5 The initial rate of different concentrations of dbm

The experiments were conducted in the different concentrations of **dbm**. The procedure was same to that described in section 3.4. The plot showed that the initial rate was slightly increased with the decreasing amount of **dbm** (Figure S10).

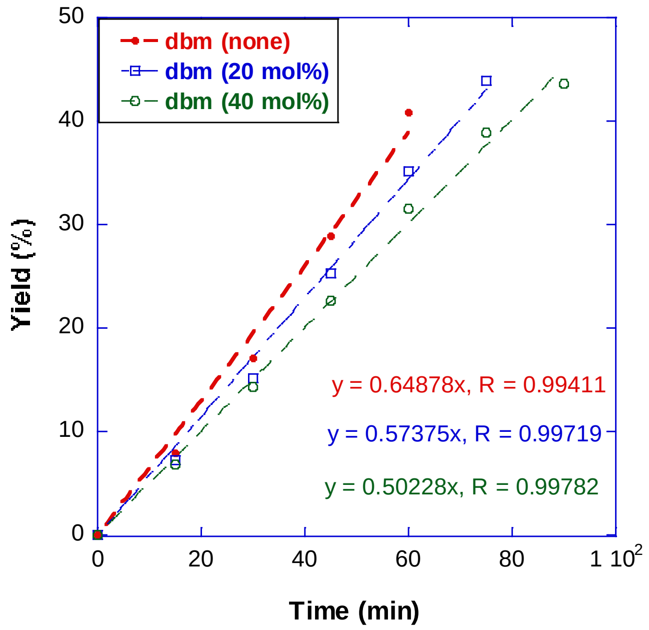
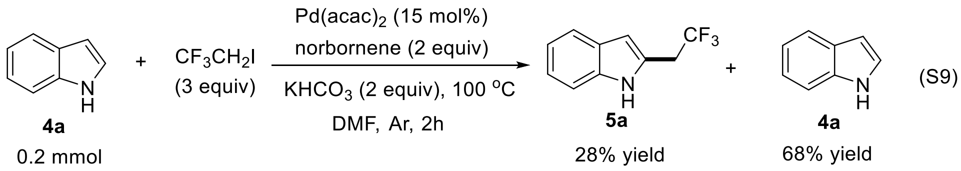



**Figure S10.**The reaction rate dependence on the concentrations of **dbm**

### 3.6 ESI-Mass studies.

ESI-MS(/MS) spectra were recorded on a Thermo TSQ (Thermo Finnigan, Quantum Access TM) triple-quadrupole mass spectrometer equipped with a standard ESI ion source.[8,9,10] The basic ESI conditions were: vacuum, $2.8\times10^{-6}$ torr; spray voltage, 2500~3000 V; capillary temperature, 270°C; sheath gas pressure, 5 arb. units; aux gas pressure, 2 arb. units; the collision energy ranged from 5 to 30 eV depending on the dissociation capability of the precursor ions. Data acquisition and analysis were done with the Xcalibur (version 2.0, Thermoquest Finnigan) software package. The experimental results showed that the negative ion mode at 2500~3000 V is suitable for the characterization of the Pd-complexes of this research. When the reaction finished, the reaction solution was cooled to room temperature and released the high pressure vessel. The concentrated reaction solutions were first filtered by PTFE Syringe Filter and then diluted with 100 times with DMF before ESI-MS analysis. The injection speed of the reaction solution was set to 5 μL/min.

***Notes***: The ions containing Pd gave their representative isotopic clusters in ESI MS spectra, thus the *m/z* values of these Pd complex ions shown in this paper are the peaks with their highest abundance.



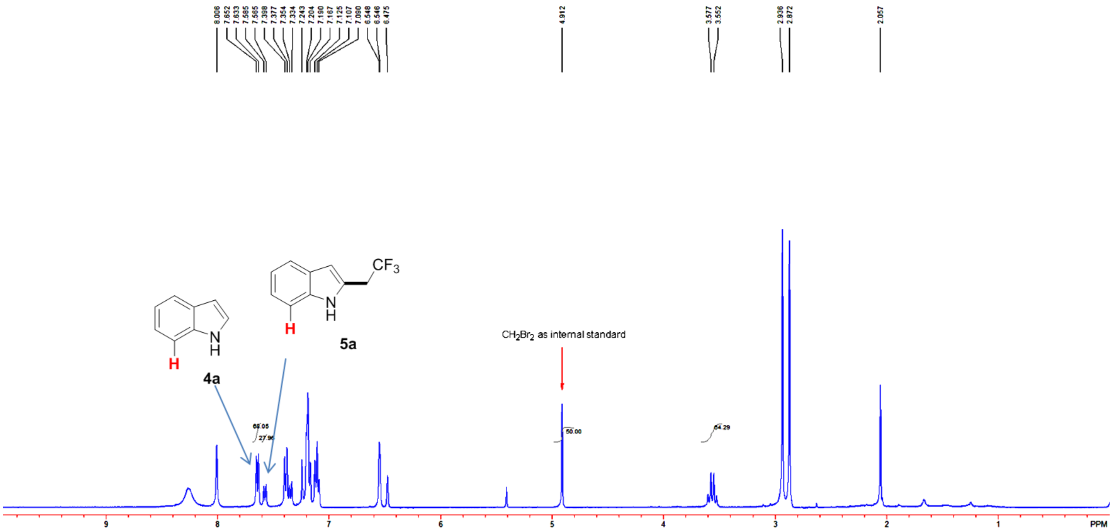
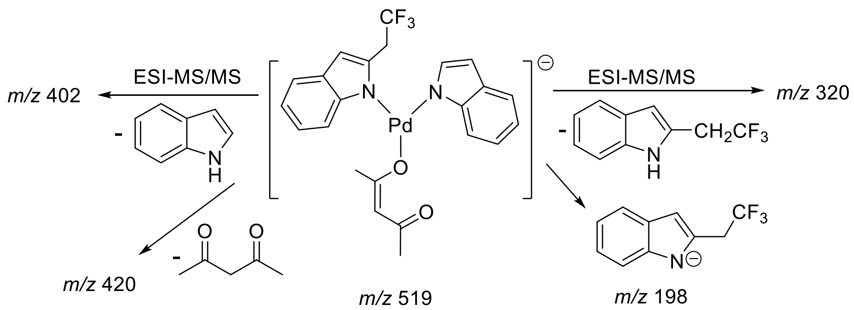




**Figure S11.** The crude $^{1}H$ NMR spectrum of the reaction in S9.

The reaction was conducted under standard condition but without **dbm** for 2 hours (eq S9). After that, the reaction solution was cooled to room temperature and filtered through PTFE Syringe Filter. The clear solution was analyzed by $^{1}H$ NMR and ESI-MS, which showed that the mixture contains product **5a** in 28% yield and substrate **4a** in 68% yield. The crude $^{1}H$ NMR spectrum and ESI-MS spectra are listed in Figure S11 and S12.

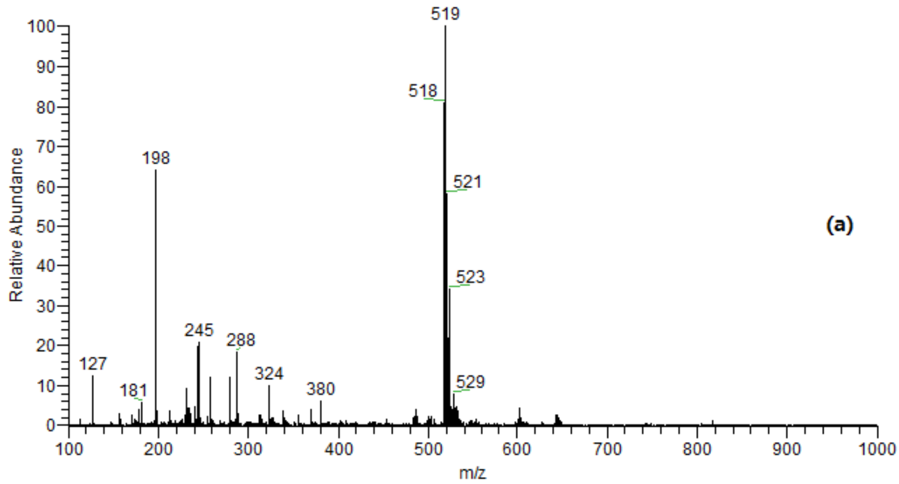
The proposed structures of the anionic Pd complex at *m/z* 519 from ESI studies of reaction solution and the proposed dissociation pathways for structural characterizations are listed in below (Scheme S1).

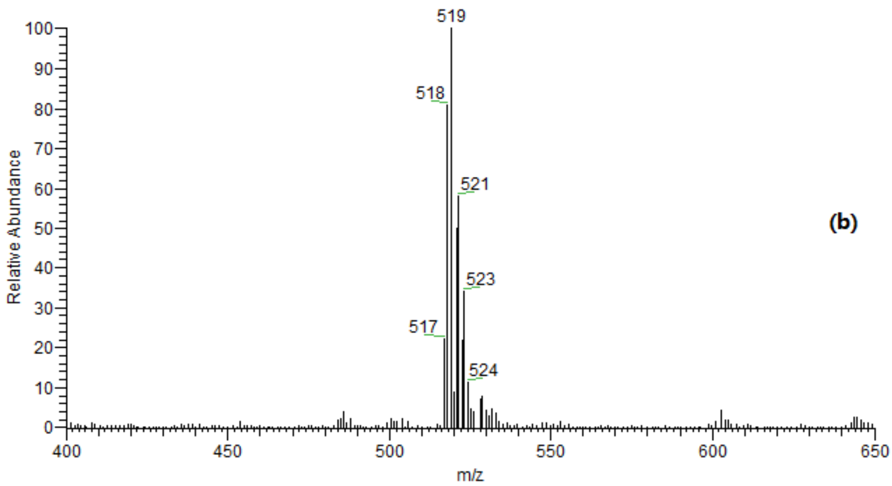



**Scheme S1.** The possible dissociation pathway of the anionic Pd complex at *m/z* 519 from ESI-MS studies of the reaction solution (eq S9).

In order to help understanding the catalytic system, alternative simple physical mixture of 0.06 mmol **5a** (30% yield), 0.14 mmol **4a** (70% yield), $Pd(acac)_2$ and $KHCO_3$ in DMF was heated for two hours, then the mixture reaction solution was monitored by ESI-MS at the same condition, the obvious different spectra was observed, which listed in Figure S12. The significant observations between catalytic reaction and physical mixture solution revealed that $Pd(acac)_2$ does not existed in the catalytic system.

ESI-MS Spectra:



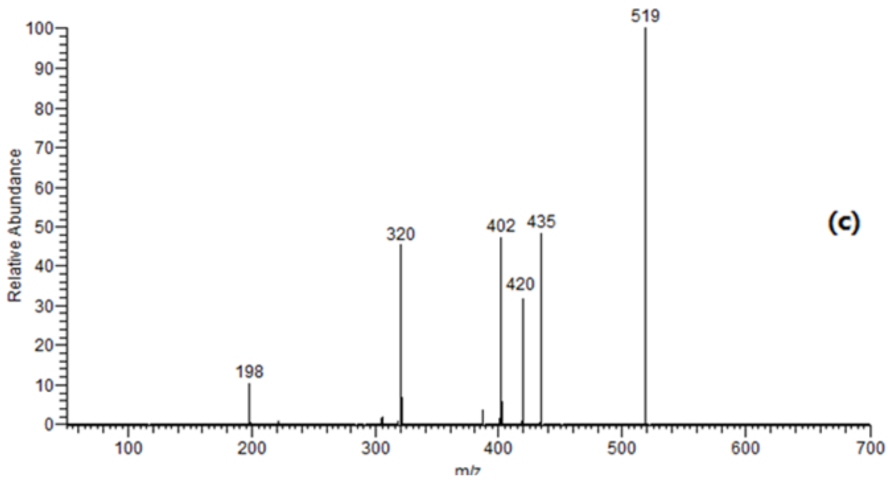
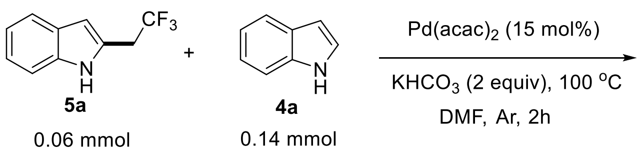



**Figure S12.** (a) The negative ion mode ESI-MS spectrum for the diluted reaction solution (eq S9). (b) The isotopic distribution of the anionic Pd complex at *m/z* 519 in the expanded ESI-MS spectrum. (c) ESI-MS/MS spectrum for the anionic Pd complex at *m/z* 519.




(S10)

To a dried 4 mL glass sealed tube, substrate **4a** (16.4 mg, 0.14 mmol), **5a** (11.9 mg, 0.06 mmol), Pd(acac)$_2$ (9.1 mg, 0.03 mmol, 15 mol %) and $KHCO_3$ (40.0 mg, 0.4 mmol, 2 equiv) were dissolved in dry DMF (1.0 mL)under Ar atmosphere. Then the mixture was stirred at room temperature for 5 minutes. The sealed tube was subsequently immersed in a preheated oil bath at 100 $^{o}$C for 2 hours. After that, the reaction was cooled to room temperature and the mixture was filtered through PTFE Syringe Filter. The clear solution was diluted 100 times with DMF and then analyzed by ESI-MS. The ESI-MS analysis results are listed in below Figure S13.

ESI-MS Spectra:

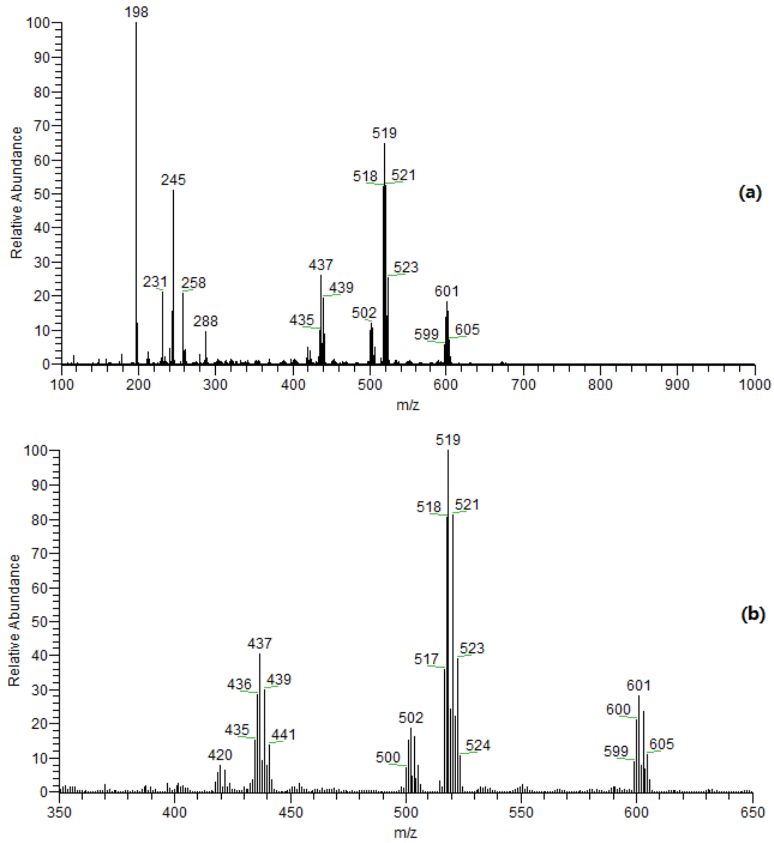
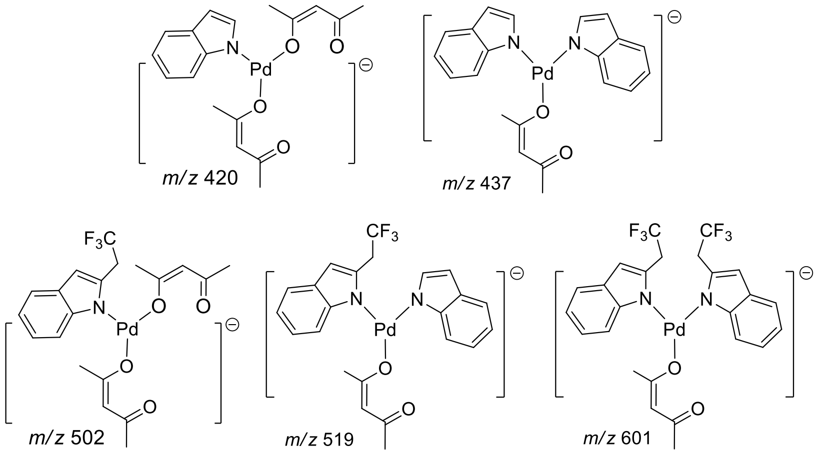



**Figure S13.** (a) The negative ion mode ESI-MS spectrum for the diluted reaction solution (eq S10). (b) the isotopic distributions of the anionic Pd complexes in the expanded ESI-MS spectrum.




**Scheme S2.** The possible structures of the anionic Pd complexes at *m/z* 420, 437, 502, 519 and 601 from ESI-MS studies of the reaction solution (eq S10).

## 4. DFT Calculation

### 4.1. Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

### 4.2. Computational Methods

Density functional theory (DFT) investigations were performed to delineate the detailed mechanism of this palladium-catalyzed C-H bond trifluoroethylation reaction. All density functional theory calculations were carried out with the Gaussian 09 programs. Geometry optimization and unscaled harmonic vibration frequency [S11] calculation were carried out using the B3LYP functional, [12] and a mixed basis set (SDD [13] for palladium and 6-31+G(d) for other atoms). The solvent effects were considered by single point energy calculations on the gas-phase stationary points using M11-L [14] functional with the 6-311+G(d,p) basis set (SDD for palladium atoms) in a SMD continuum solvation model. [15] The energies given in this work are M11-L calculated Gibbs free energies in DMF solvent.

### 4.3. Absolute Calculation Energies, Enthalpies, and Free Energies

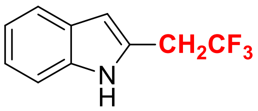
| Geometry | $E_{(elec\text{-}B3LYP)}$[1] | $E_{(solv,\ M11\text{-}L)}$[2] | $G_{(corr\text{-}B3LYP)}$[3] | $H_{(corr\text{-}B3LYP)}$[4] | IF[5] |
|---|---|---|---|---|---|
| **int.V** | -836.344691 | -836.586992 | 0.185318 | 0.250071 | - |
| **int.VI** | -1109.087971 | -1109.361183 | 0.333847 | 0.412335 | - |
| **TS1** | -1109.067382 | -1109.340888 | 0.335262 | 0.411179 | -245.25 |
| **int.I-dk** | -1109.086484 | -1109.352509 | 0.338359 | 0.414112 | - |
| **4a** | -363.809320 | -363.809320 | 0.099648 | 0.137254 | - |
| **TS2** | -1373.566555 | -1373.948417 | 0.352876 | 0.440262 | -545.76 |
| **5a** | -740.164851 | -740.164851 | 0.125784 | 0.175896 | - |
| **int.II-dk** | -1108.591707 | -1108.924370 | 0.324462 | 0.399947 | - |
| **TS3** | -1496.944991 | -1497.323363 | 0.356291 | 0.451012 | -232.99 |
| **int.IV** | -1485.424972 | -1485.694704 | 0.362792 | 0.450778 | - |
| **TS4** | -1485.402294 | -1485.673166 | 0.363991 | 0.449656 | -339.70 |
| **int.VII** | -1485.450910 | -1485.734179 | 0.366106 | 0.452414 | - |
| **TS5** | -1485.420868 | -1485.704810 | 0.362329 | 0.449689 | -257.67 |
| **int.VIII** | -1485.443950 | -1485.723278 | 0.361288 | 0.450845 | - |
| **int.IX** | -1576.548898 | -1576.857348 | 0.335739 | 0.428136 | - |
| **TS6** | -1576.505732 | -1576.806328 | 0.331734 | 0.423167 | -1422.4 |
| **int.XII** | -836.347470 | -836.598221 | 0.186752 | 0.249826 | - |
| **int.X** | -1151.637169 | -1151.940583 | 0.252033 | 0.330936 | - |
| **TS7** | -1151.607627 | -1151.909079 | 0.25335 | 0.329158 | -205.45 |
| **int.XI** | -1151.655070 | -1151.958766 | 0.255607 | 0.330857 | - |
| **TS8** | -1576.513167 | -1576.799347 | 0.329763 | 0.422229 | -1263.3 |
| **TS9** | -1576.501166 | -1576.799019 | 0.329441 | 0.329441 | -1025.3 |
| **Norborn.** | -272.722693 | -272.760510 | 0.125198 | 0.159861 | - |
| **$HCO_3^-$** | -264.420220 | -264.583716 | 0.000483 | 0.030723 | - |
| **$H_2O$** | -76.407024 | -76.450265 | 0.003474 | 0.024919 | - |
| **$CO_2$** | -188.577570 | -188.592551 | -0.009098 | 0.015204 | - |
| **acac$^-$** | -345.208235 | -345.356111 | 0.075945 | 0.118366 | - |
| **$CF_3CH_2I$** | -388.354364 | -388.354364 | 0.010711 | 0.050002 | - |
| **$I^-$** | -11.518910 | -11.518910 | -0.016848 | 0.00236 | - |

[1]The electronic energy calculated by B3LYP in gas phase. [2]The electronic energy calculated by M11-L in toluene solvent. [3]The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. [4]The thermal correction to enthalpy calculated by B3LYP in gas phase. [5]The B3LYP calculated imaginary frequencies for the transition states.

### 4.4. B3LYP Geometries for All the Optimized Compounds and Transition States

Attached in the end of SI.

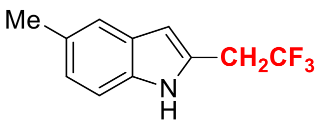
## 5. New Compounds Characterization




**5a**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by y column chromatography on silica gel with petroleum ether/ethyl acetate (25:1 to 20:1) to afford the product **5a** in 78% yield (31.1 mg).

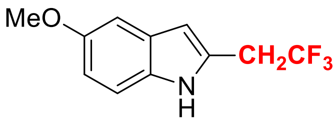
$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.94 (br, 1H), 7.58 (d, $J$ = 7.6 Hz, 1H), 7.30 (d, $J$ = 8.4 Hz, 1H), 7.19 (t, $J$ = 7.6 Hz, 1H), 7.12 (t, $J$ = 7.2 Hz, 1H), 6.46 (s, 1H), 3.50 (q, $J$ = 10.4 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 136.5, 128.0, 126.5, 125.1 (q, $J$ = 275.2 Hz), 122.5, 120.5, 120.2, 110.8, 104.4, 33.7 (q, $J$ = 31.1 Hz). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.3 (t, $J$ = 10.5 Hz). HRMS: m/z (EI) calculated [$M^+$]: 199.0609, measured: 199.0612.




**5b**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (25:1 to 20:1) to afford the product **5b** in 76% yield (32.4 mg).

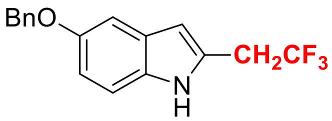
$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.97 (br, 1H), 7.37 (s, 1H), 7.23 (d, $J$ = 7.2 Hz, 1H), 7.02 (d, $J$ = 7.6 Hz, 1H), 6.40 (s, 1H), 3.55 (q, $J$ = 10.4 Hz, 2H), 2.43 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 134.8, 129.4, 128.2, 126.6, 125.1 (q, $J$ = 276.0 Hz), 124.1, 120.1, 110.4, 103.9, 33.8 (q, $J$ = 31.1 Hz), 21.4. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.4 (t, $J$ = 10.2 Hz). HRMS: m/z (EI) calculated [$M^+$]: 213.0765, measured: 213.0769.



**5c**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (30:1 to 25:1) to afford the product **5c** in 82% yield (37.8 mg).

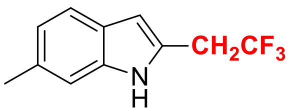
$^1$H NMR (400 MHz, $CDCl_3$) δ 7.98 (br, 1H), 7.23 (d, *J* = 9.2 Hz, 1H), 7.04 (s, 1H), 6.87 (dd, *J* = 8.8,2.4 Hz, 1H), 6.41 (s, 1H), 3.84 (s, 3H), 3.54 (q, *J* = 10.4 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 154.3, 131.6, 128.4, 127.3, 125.1 (q, *J* = 275.6 Hz), 112.7, 111.6, 104.0, 102.1, 55.8, 33.6 (q, *J* = 31.5 Hz). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.4 (t, *J* = 10.5 Hz). HRMS: m/z (EI) calculated [$M^+$]: 229.0714, measured: 229.0715.



**5d**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (20:1 to 15:1) to afford the product **5d** in 75% yield (45.7 mg).

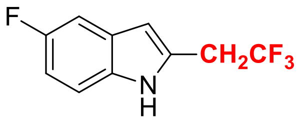
$^1$H NMR (400 MHz, $CDCl_3$) δ 7.95 (br, 1H), 7.46 (d, *J* = 7.2 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 7.2 Hz, 1H), 7.21 (d, *J* = 9.6 Hz, 1H), 7.11 (d, *J* = 2.0 Hz, 1H), 6.94 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.39 (s, 1H), 5.08 (s, 2H), 3.50 (q, *J* = 10.4 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.5, 137.5, 131.8, 128.5, 128.4, 127.8, 127.5, 127.3, 125.1 (q, *J* = 275.6 Hz), 113.5, 111.6, 104.2, 103.8, 70.8, 33.7 (q, *J* = 31.1 Hz). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.3 (t, *J* = 10.5 Hz). HRMS: m/z (EI) calculated [$M^+$]: 305.1027, measured: 305.1026.



**5e**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (30:1 to 25:1) to afford the product **5e** in 74% yield (31.7 mg).

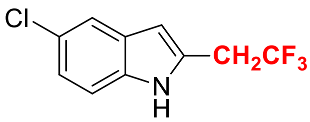
$^1$H NMR (400 MHz, $CDCl_3$) δ 7.93 (br, 1H), 7.46 (d, $J$ = 8.0 Hz, 1H), 7.14 (s, 1H), 6.95 (d, $J$ = 8.4 Hz, 1H), 6.42 (s, 1H), 3.54 (q, $J$ = 10.4 Hz, 2H), 2.45 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 136.9, 132.4, 125.8, 125.7, 125.1 (q, $J$ = 275.5 Hz), 121.9, 120.1, 110.7, 104.2, 33.7 (q, $J$ = 31.1 Hz), 21.7. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.4 (t, $J$ = 10.2 Hz). HRMS: m/z (EI) calculated [$M^+$]: 213.0765, measured: 213.0764.




**5f**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (30:1 to 25:1) to afford the product **5f** in 78% yield (33.9 mg).

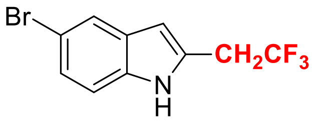
$^1$H NMR (400 MHz, $CDCl_3$) δ 8.09 (br, 1H), 7.27 (t, $J$ = 4.4 Hz, 1H), 7.23 (dd, $J$ = 9.6, 2.8 Hz, 1H), 7.23 (dt, $J$ = 9.2, 2.4 Hz, 1H), 6.45 (s, 1H), 3.57 (q, $J$ = 10.4 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 158.0 (d, $J$ = 233.8 Hz), 133.0, 128.3, 128.2 125.0 (q, $J$ = 275.6 Hz), 111.5 (d, $J$ = 9.5 Hz), 110.9 (d, $J$ = 26.2 Hz), 105.3 (d, $J$ = 23.5 Hz), 104.5 (d, $J$ = 4.2 Hz), 33.8 (q, $J$ = 31.1 Hz). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.3 (t, $J$ = 10.5 Hz), -124.2 (dt, $J$ = 9.4, 4.5 Hz). HRMS: m/z (EI) calculated [$M^+$]: 217.0515, measured: 217.0517.




**5g**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (25:1 to 20:1) to afford the product **5g** in 80% yield (37.4 mg).

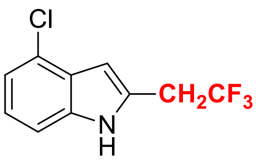
$^{1}H$ NMR (400 MHz, $CDCl_3$) δ 8.13 (br, 1H), 7.55 (s,1H), 7.27 (d, *J* = 8.8 Hz, 1H), 7.16 (dd, *J* = 8.8, 1.6 Hz, 1H), 6.44 (s, 1H), 3.58 (q, *J* = 10.4 Hz, 2H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 134.8, 129.0, 128.0, 125.9, 125.0 (q, *J* = 275.6 Hz), 122.9, 119.9, 111.8, 104.1, 33.7 (q, *J* = 31.8 Hz). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -65.3 (t, *J* = 10.2 Hz). HRMS: m/z (EI) calculated [$M^+$]: 233.0219, measured: 233.0218.




**5h**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (30:1 to 25:1) to afford the product **5h** in 66% yield (36.6 mg).

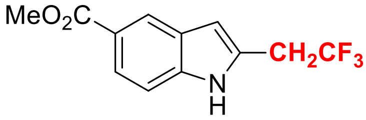
$^{1}H$ NMR (400 MHz, $CDCl_3$) δ 8.15 (br, 1H), 7.71 (s, 1H), 7.22-7.30 (m, 2H), 6.44 (s, 1H), 3.58 (q, *J* = 10.4 Hz, 2H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 135.1, 129.7, 127.9, 125.4, 124.9 (q, *J* = 275.8 Hz), 123.0, 113.4, 112.2, 104.0, 33.7 (q, *J* = 31.9 Hz). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -65.2 (t, *J* = 10.9 Hz). HRMS: m/z (EI) calculated [$M^+$]: 276.9714, measured: 276.9717.




**5i**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (25:1 to 20:1) to afford the product **5i** in 80% yield (37.3 mg).

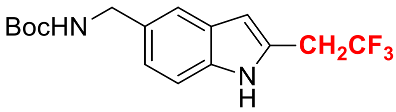
$^{1}H$ NMR (400 MHz, $CDCl_3$) δ 8.20 (br, 1H), 7.23-7.27 (m, 1H) 7.11-7.13 (m,2H), 6.60 (s, 1H), 3.59 (q, *J* = 10.4 Hz, 2H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 137.1, 127.2, 126.9, 125.8, 124.9 (q, *J* = 275.7 Hz), 123.2, 120.0, 109.5, 103.1, 33.7 (q, *J* = 31.8 Hz). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -65.3 (t, *J* = 10.2 Hz). HRMS: m/z (EI) calculated [$M^+$]: 233.0219, measured: 233.0225.



**5j**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (20:1 to 12:1) to afford the product **5j** in 74% yield (38.0 mg).

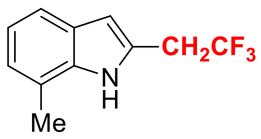
$^1$H NMR (400 MHz, $CDCl_3$) δ 8.43 (br, 1H), 8.36 (s, 1H), 7.92 (d, $J$ = 8.4 Hz, 1H), 7.37 (d, $J$ = 8.8 Hz, 1H), 6.59 (s, 1H), 3.94 (s, 3H), 3.61 (q, $J$ = 10.4 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.1, 139.1, 128.1, 127.6, 124.9 (q, $J$ = 275.6 Hz),123.9, 123.5, 122.3, 110.6, 105.6, 51.9, 33.7 (q, $J$ = 31.1 Hz). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.2 (t, $J$ = 10.2 Hz). HRMS: m/z (EI) calculated [$M^+$]: 257.0664, measured: 257.0671.



**5k**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1 to 4:1) to afford the product **5k** in 63% yield (44.2 mg).

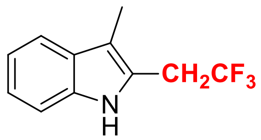
$^1$H NMR (400 MHz, $CDCl_3$) δ 8.69 (br, 1H), 7.44 (s, 1H), 7.23 (d, $J$ = 8.4 Hz, 1H), 7.06 (d, $J$ = 8.0 Hz, 1H), 6.40 (s, 1H), 4.93 (s, 1H), 4.36 (d, $J$ = 5.6 Hz, 2H), 3.50 (q, $J$ = 10.4 Hz, 2H), 1.47 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 156.1, 135.9, 130.3, 128.2, 127.4, 125.1 (q, $J$ = 275.6 Hz), 122.3, 119.4, 111.2, 103.9, 79.5, 45.2, 33.5 (q, $J$ = 31.0 Hz), 20.4. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.4 (t, $J$ = 10.5 Hz). HRMS: m/z (EI) calculated [$M+NH_4$]$^+$: 351.1291, measured: 351.1292.



**5l**

The reaction was conducted with general procedure in 0.2 mmol scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (40:1 to 30:1) to afford the product **5l** in 13% yield (5.6 mg).

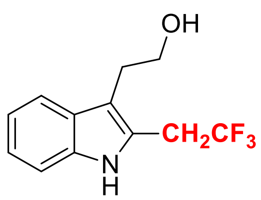
$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.99 (br, 1H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.07- 7.00 (m,2H), 6.50 (s, 1H), 3.61 (q, *J* = 10.8 Hz, 2H), 2.50 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 136.1, 127.5, 126.2, 125.1 (q, *J* = 275.5 Hz), 123.0, 120.4, 120.0, 118.2, 105.0, 33.8 (q, *J* = 31.1 Hz), 16.6. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.4 (t, *J* = 10.2 Hz). HRMS: m/z (ESI) calculated $[M+H]^+$: 213.0838, measured:.214.0839.



**5m**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (30:1 to 25:1) to afford the product **5m** in 80% yield (34.1 mg).

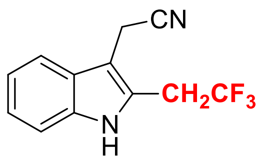
$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.89 (br, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.13 (t, *J* = 7.2 Hz, 1H), 3.55 (q, *J* = 10.4 Hz, 2H), 2.29 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 135.8, 128.7, 128.5, 125.4 (q, *J* = 276.3 Hz), 122.6, 119.5, 118.9, 111.8, 110.7, 31.5 (q, *J* = 31.5 Hz), 8.39. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.1 (t, *J* = 10.5 Hz). HRMS: m/z (EI) calculated $[M^+]$: 213.0765, measured: 213.0766 .



**5n**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (3:1 to 1:1) to afford the product **5n** in 58% yield (28.2 mg).

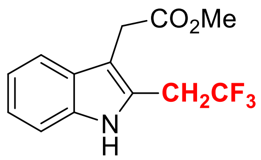
$^1$H NMR (400 MHz, $CDCl_3$) δ 8.18 (br, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.13 (t, *J* = 7.2 Hz, 1H), 3.83 (t, *J* = 6.4 Hz, 2H), 3.55 (q, *J* = 10.4 Hz, 2H), 2.98 (t, *J* = 6.4 Hz, 2H), 1.69 (s, 1H) . $^{13}$C NMR (100 MHz, $CDCl_3$) δ 136.0, 127.6, 125.2 (q, *J* = 276.4 Hz), 124.2, 122.7, 119.8, 118.8, 112.2, 110.9, 62.6, 31.4 (q, *J* = 31.2 Hz), 27.5. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -64.9 (t, *J* = 10.5 Hz). HRMS: m/z (EI) calculated [$M^+$]: 243.0871, measured: 243.0874.




**5o**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (10:1 to 5:1) to afford the product **5o** in 66% yield (31.4 mg).

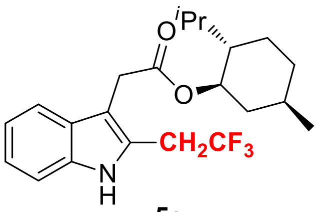
$^1$H NMR (400 MHz, $d_6$-Acetone) δ 10.5 (br, 1H), 7.71 (dd, *J* = 8.0, 0.4 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.21 (dt, *J* = 7.2, 0.8 Hz, 1H), 7.15 (dt, *J* = 7.6, 0.8 Hz, 1H), 4.07 (s, 1H), 3.96 (q, *J* = 10.8 Hz, 2H). $^{13}$C NMR (100 MHz, $d_6$-Acetone) δ 136.2, 126.9, 125.8 (q, *J* = 275.5 Hz), 125.2, 122.7, 119.8, 118.2, 118.0, 111.4, 104.4, 30.5 (q, *J* = 31.1 Hz), 12.0. $^{19}$F NMR (376 MHz, $d_6$-Acetone) δ -65.7 (t, *J* = 10.2 Hz). HRMS: m/z (EI) calculated [$M^+$]:238.0718, measured: 238.0721.




**5p**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (15:1 to 8:1) to afford the product **5p** in 76% yield (41.2 mg).

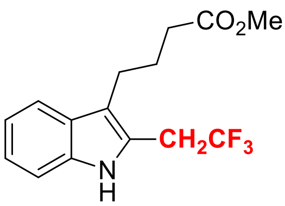
$^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.17 (br, 1H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.21 (dt, *J* = 7.2, 1.6 Hz, 1H), 7.15 (dt, *J* = 8.4, 1.6 Hz, 1H), 3.74 (s, 2H), 3.67 (s, 3H), 3.56 (q, *J* = 10.4 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 172.0, 135.7, 127.5, 125.2 (q, *J* = 276.1 Hz), 124.5, 122.8, 120.1, 118.8, 110.9, 108.6, 52.1, 31.4 (q, *J* = 31.3 Hz), 29.9. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -64.9 (t, *J* = 10.5 Hz). HRMS: m/z (EI) calculated [$M^+$]: 271.0820, measured: 271.0824.




**5q**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1 to 4:1) to afford the product **5q** in 58% yield (45.9 mg).

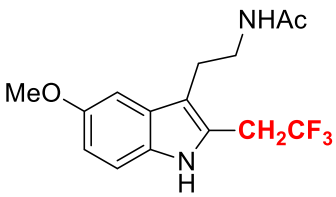
$^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.17 (br, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.12 (td, *J* = 6.8, 0.8 Hz, 1H), 7.12 (td, *J* = 7.6, 0.8 Hz, 1H), 4.61 (td, *J* = 10.8, 4.4 Hz, 1H), 3.65 (s, 2H), 3.35 (q, *J* = 10.8 Hz, 2H), 1.91-1.88 (m, 1H), 1.65-1.54 (m, 3H), 1.39-1.23 (m, 2H), 0.99-0.84 (m, 2H), 0.81-0.74 (m, 1H), 0.80 (d, *J* = 6.4 Hz, 3H), 0.73 (d, *J* = 7.2 Hz, 3H), 0.58 (d, *J* = 7.2 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 171.3, 135.7, 127.6, 126.6 (q, *J* = 276.1 Hz), 124.4, 122.7, 119.9, 118.9, 110.9, 108.8, 74.9, 47.0, 40.7, 34.2, 31.3, 31.2 (q, *J* = 31.3 Hz), 30.4, 26.1, 23.3, 21.9, 20.6, 16.1. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -64.9 (t, *J* = 10.5 Hz). HRMS: m/z (ESI) calculated [$M+NH_4$]$^+$: 413.2410, measured: 413.2414.




**5r**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (15:1 to 10:1) to afford the product **5r** in 56% yield (33.5 mg).

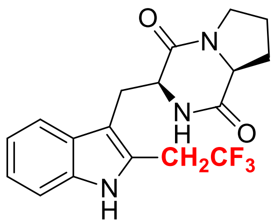
$^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.06 (br, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 7.19 (t, *J* = 8.0 Hz, 1H), 7.11 (t, *J* = 6.8 Hz, 1H), 3.66 (s, 3H), 3.53 (q, *J* = 10.4 Hz, 2H), 2.77 (t, *J* = 7.6 Hz, 2H), 2.36 (t, *J* = 7.2 Hz, 2H), 1.95-2.02 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 174.1, 135.9, 127.6, 125.3 (q, *J* = 275.9 Hz), 122.9, 122.5, 119.6, 119.0, 115.4, 110.8, 51.5, 33.3, 31.3 (q, *J* = 30.4 Hz), 25.6, 23.2. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -64.9 (t, *J* = 10.5 Hz). HRMS: m/z (EI) calculated [$M^+$]: 299.1133, measured: 299.1126.




**5s**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1 to 4:1) to afford the product **5s** in 58% yield (36.5 mg).

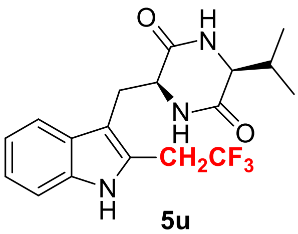
$^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.30 (br, 1H), 7.24 (d, *J* = 9.2 Hz, 1H), 7.03 (s, 1H), 6.88 (dd, *J* = 8.4, 1.2 Hz, 1H), 5.64 (s, 1H), 3.85 (s, 3H), 3.51-3.59 (m, 4H), 2.92 (t, *J* = 6.4 Hz, 2H), 1.91 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 170.4, 154.1, 131.2, 127.9, 125.2 (q, *J* = 275.7 Hz), 124.5, 112.7, 112.3, 111.8, 100.5, 55.8, 39.7, 31.3 (q, *J* = 30.8 Hz), 30.8, 24.1, 23.1. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -64.8 (t, *J* = 10.2 Hz). HRMS: m/z (EI) calculated [$M^+$]: 314.1242, measured: 314.1238 .




**5t**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1 to 4:1) to afford the product **5t** in 38% yield (27.8 mg).

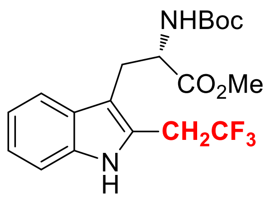
$^1$H NMR (400 MHz, $CDCl_3$) δ 8.38 (br, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 1H), 5.65 (s, 1H), 4.41 (dd, *J* = 10.8, 4.0 Hz, 1H), 4.08 (t, *J* = 8.0 Hz, 1H), 3.72-3.56 (m, 5H), 3.01 (dd, *J* = 13.2, 10.4 Hz, 1H), 2.35-2.33 (m, 1H), 2.07-1.98 (m, 2H), 1.96-1.87 (m, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 169.4, 165.4, 136.1, 127.0, 125.1 (q, *J* = 276.1 Hz), 125.0, 123.4, 120.5, 118.4, 111.3, 109.8, 59.2, 54.6, 45.6, 31.4 (q, *J* = 31.2 Hz), 28.3, 25.5, 22.6. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -64.6 (t, *J* = 10.9 Hz). HRMS: m/z (ESI) calculated $[M+H]^+$: 366.1424, measured: 366.1425.




**5u**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1 to 4:1) to afford the product **5u** in 33% yield (24.3 mg).

$^1$H NMR (400 MHz, $d_6$-DMSO) δ 11.02 (br, 1H), 8.14 (s, 1H), 7.97 (s, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.95 (t, *J* = 7.6 Hz, 1H), 4.16 (s, 1H), 3.91-3.72 (m, 2H), 3.41 (s, 1H), 3.28 (dd, *J* = 14.4, 3.6 Hz, 1H), 3.08 (dd, *J* = 14.4, 3.6 Hz, 1H), 1.42-1.36 (m, 1H), 0.51 (d, *J* = 7.2 Hz, 3H), 0.06 (d, *J* = 7.2 Hz, 3H). $^{13}$C NMR (100 MHz, $d_6$-DMSO) δ 168.0, 166.8, 136.1, 128.6, 126.2 (q, *J* = 275.4 Hz), 125.9, 121.9, 119.7, 119.2, 111.2, 109.4, 59.7, 55.7, 31.9, 30.6 (q, *J* = 29.6 Hz), 28.0, 18.7, 16.5. $^{19}$F NMR (376 MHz, $d_6$-DMSO) δ -63.7 (t, *J* = 10.5 Hz). HRMS: m/z (ESI) calculated $[M+H]^+$: 368.1850, measured: 368.1850.

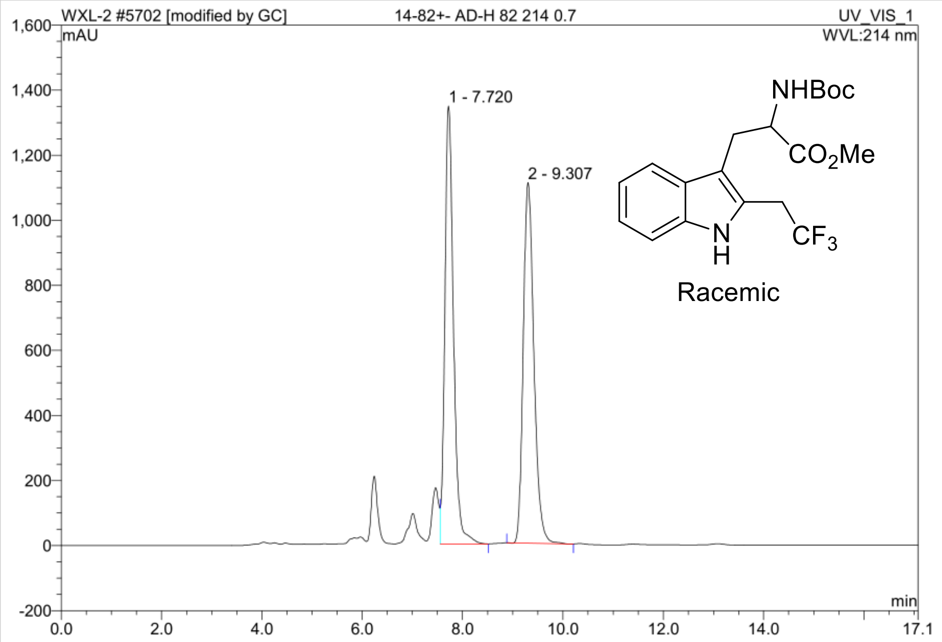



**5v**

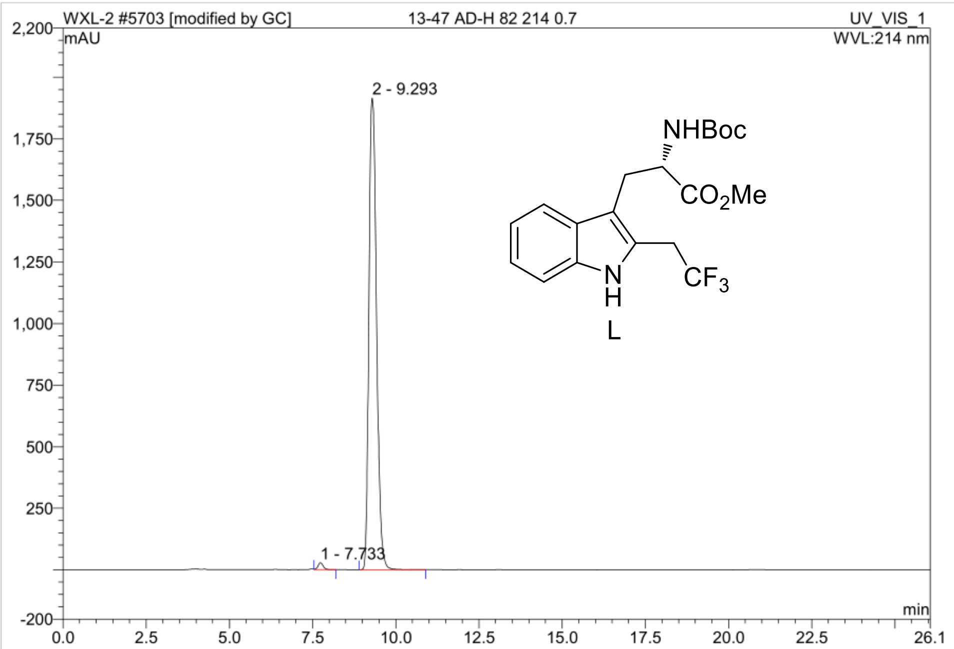
The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (15:1 to 10:1) to afford the product **5v** in 56% yield (44.8 mg, 98% ee).

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.43 (br, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.10 (t, *J* = 7.2 Hz, 1H), 5.17 (d, *J* = 7.6 Hz, 1H), 4.62 (d, *J* = 7.6 Hz, 1H), 3.61 (s, 3H), 3.53 (q, *J* = 10.4 Hz, 2H), 3.27 (d, *J* = 3.6 Hz, 2H), 1.42 (s, 9H) . $^{13}$C NMR (100 MHz, $CDCl_3$) δ 172.5, 155.1, 135.8, 127.7, 125.2 (q, *J* = 275.7 Hz), 124.7, 122.6, 119.8, 118.8, 110.9, 110.0, 80.0, 54.0, 52.3, 31.2 (q, *J* = 30.8 Hz), 27.0. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -64.5 (t, *J* = 10.5 Hz). HRMS: m/z (EI) calculated [$M^+$]: 400.1610, measured: 400.1604.

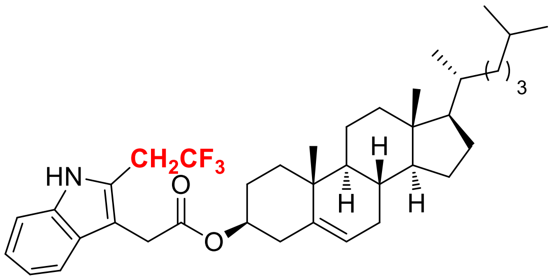
HPLC (AD-H, 0.46*25 cm, 5 μm, hexane / isopropanol = 8/2, flow 0.7 mL/min, detection at 214 nm) retention time = 17.73 min (minor) and 9.29 min (major).




| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 7.72 | n.a. | 1347.324 | 269.592 | 49.78 | n.a. | MB* |
| 2 | 9.31 | n.a. | 1108.929 | 272.014 | 50.22 | n.a. | BMB* |
| Total: | | | 2456.253 | 541.606 | 100.00 | 0.000 | |



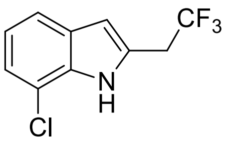

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 7.73 | n.a. | 28.354 | 5.151 | 1.00 | n.a. | MB* |
| 2 | 9.29 | n.a. | 1916.224 | 512.130 | 99.00 | n.a. | BMB |
| Total: | | | 1944.578 | 517.281 | 100.00 | 0.000 | |




**5w**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1 to 4:1) to afford the product **5w** in 51% yield (61.0 mg).

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.17 (br, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.15 (t, *J* = 7.2 Hz, 1H), 5.34 (d, *J* = 3.6 Hz, 1H), 4.62-4.57 (m, 1H), 3.71 (s, 2H), 3.36 (q, *J* = 10.4 Hz, 2H), 2.30 (d, *J* = 7.6 Hz, 2H), 2.02-1.94 (m, 2H), 1.85-1.82 (m, 3H), 1.60-0.96 (m, 21H), 1.01 (s, 3H), 0.91 (d, *J* = 6.0 Hz, 3H), 0.87 (d, *J* = 6.8 Hz, 6H), 0.68 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 170.8, 139.5, 135.7, 127.6, 125.3 (q, *J* = 276.6 Hz), 124.3, 122.8, 122.7, 120.0, 119.0, 110.8, 108.9, 74.7, 56.6, 56.1, 49.9, 42.3, 39.7, 39.5, 37.9, 36.9, 36.5, 36.2, 35.8, 31.9, 31.8, 31.4 (q, *J* = 31.0 Hz), 30.5, 28.2, 28.0, 27.7, 24.2, 23.8, 22.8, 22.5, 21.0, 19.3, 18.7, 11.8. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -64.8 (t, *J* = 10.2 Hz). HRMS: m/z (ESI) calculated $[M+NH_4]^+$: 643.4445, measured: 643.4445.




**5x**

The reaction was conducted with general procedure in 0.2 mmol Scale. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (30:1 to 25:1) to afford the product **5s** in 30% yield (14.0 mg).

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.27 (br, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.20 (d, *J* =7.6 Hz, 1H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.54 (s, 1H), 3.61 (q, *J* = 10.4 Hz, 2H). $^{13}$C NMR (150 MHz, $CDCl_3$) δ 133.8, 129.3, 127.4, 124.9 (q, *J* = 275.5 Hz), 121.9, 121.0, 119.1, 116.3, 105.4, 33.7 (q, *J* = 31.2 Hz). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -65.3 (t, *J* = 10.5

Hz). HRMS: m/z (EI) calculated [$M^+$]:233.0219, measured: 233.0213 .

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## Appendix for DTF calculation:

## 4.3. B3LYP Geometries for All the Optimized Compounds and Transition States

**int.V**

| | | | |
|---|---|---|---|
| C | -3.42698900 | -0.05482500 | -0.60443500 |
| C | -2.28978200 | -0.23540000 | 0.23048400 |
| C | -2.28787400 | 0.18280600 | 1.56078600 |
| C | -3.44475300 | 0.78796900 | 2.06100800 |
| C | -4.58059400 | 0.95117600 | 1.25303700 |

| | | | |
|---|---|---|---|
| C | -4.58405500 | 0.52757900 | -0.07926800 |
| C | -3.05174900 | -0.57175600 | -1.90042400 |
| C | -1.76036700 | -1.01746100 | -1.78744700 |
| H | -1.41322700 | 0.03587900 | 2.18966600 |
| H | -3.46789100 | 1.12556800 | 3.09353200 |
| H | -5.47247900 | 1.40975800 | 1.67178200 |
| H | -5.47227400 | 0.65168800 | -0.69390600 |
| H | -3.67696400 | -0.63033700 | -2.78225500 |
| H | -1.13736900 | -1.47768800 | -2.54366500 |
| N | -1.27739300 | -0.87855400 | -0.49170900 |
| Pd | 0.64846000 | -0.79150000 | -0.04497900 |
| C | 3.49910300 | -0.26127800 | 0.48907100 |
| O | 2.56386300 | -1.12906800 | 0.54446900 |
| C | 3.37407900 | 1.05754700 | 0.01354900 |
| H | 4.26571700 | 1.67213600 | 0.03070500 |
| C | 2.20497700 | 1.65269800 | -0.47963000 |
| O | 1.04407900 | 1.11738700 | -0.58829500 |
| C | 2.24358400 | 3.09040600 | -0.95701600 |
| H | 3.23650500 | 3.53296000 | -0.85085400 |
| H | 1.93942400 | 3.13207200 | -2.00860100 |
| H | 1.51949700 | 3.68220900 | -0.38675600 |
| C | 4.84105800 | -0.74571900 | 0.99397800 |
| H | 5.14844800 | -1.62787400 | 0.42152800 |
| H | 5.61563600 | 0.02060800 | 0.91810800 |
| H | 4.74419200 | -1.05708800 | 2.04014900 |

**int,VI**

| | | | |
|---|---|---|---|
| C | 3.76453500 | -0.49378800 | -0.59368200 |
| C | 2.54777500 | -0.40977100 | 0.15721000 |
| C | 2.55883700 | -0.38784500 | 1.56103100 |
| C | 3.78545300 | -0.47462200 | 2.21159800 |
| C | 4.98951600 | -0.58372300 | 1.48444800 |
| C | 4.98651500 | -0.59500200 | 0.09477100 |
| C | 3.38797400 | -0.45585500 | -1.97461800 |
| C | 2.01372800 | -0.36077300 | -2.00044800 |
| H | 1.63462500 | -0.28554700 | 2.12618600 |
| H | 3.81688700 | -0.45509000 | 3.29814800 |
| H | 5.93164600 | -0.65606400 | 2.02207700 |
| H | 5.92044600 | -0.67730300 | -0.45716800 |
| H | 4.04226300 | -0.51604400 | -2.83476000 |
| H | 1.35709200 | -0.29882600 | -2.86027800 |
| N | 1.48592000 | -0.37595200 | -0.72468100 |
| C | -2.52079100 | 2.18544500 | 0.38587900 |
| C | -1.65113600 | 3.27233200 | 0.22639300 |

| | | | |
|---|---|---|---|
| H | -2.06132100 | 4.26249700 | 0.38303000 |
| C | -0.29263700 | 3.18814600 | -0.12010100 |
| O | 0.36880700 | 2.11915200 | -0.34844400 |
| C | 0.52605300 | 4.45436600 | -0.25227700 |
| H | -0.06677000 | 5.35385700 | -0.07040900 |
| H | 1.36024900 | 4.41996700 | 0.45707500 |
| H | 0.96056100 | 4.50205300 | -1.25666900 |
| C | -3.96716300 | 2.44512600 | 0.75444500 |
| H | -4.21102500 | 1.91257300 | 1.68049400 |
| H | -4.17806100 | 3.50867100 | 0.88719000 |
| H | -4.62147200 | 2.04689300 | -0.02961200 |
| Pd | -0.37188300 | 0.22086300 | -0.24902300 |
| O | -2.23012600 | 0.94467600 | 0.25018900 |
| C | -3.44268900 | -1.77176400 | -0.36509200 |
| C | -2.34791800 | -2.62061900 | -1.07397200 |
| C | -1.76953200 | -2.76269700 | 1.10864900 |
| C | -3.04023200 | -1.86343300 | 1.13873100 |
| H | -3.47313700 | -0.74263700 | -0.72170100 |
| H | -4.42240100 | -2.22779100 | -0.54613600 |
| H | -2.84873600 | -0.88269000 | 1.57403400 |
| H | -3.81720500 | -2.35735500 | 1.73265600 |
| C | -2.16458600 | -3.75811400 | -0.02369500 |
| H | -1.36628600 | -4.46204400 | -0.28069900 |
| H | -3.08736600 | -4.31383900 | 0.18448900 |
| C | -0.96578300 | -1.97543900 | -0.93893800 |
| H | -0.28701800 | -1.84977600 | -1.77442400 |
| C | -0.61181500 | -2.06491000 | 0.39040400 |
| H | 0.39311900 | -2.01562400 | 0.79359300 |
| H | -2.60026000 | -2.91819500 | -2.09424800 |
| H | -1.49671400 | -3.18870600 | 2.07658700 |

**TS1**

| | | | |
|---|---|---|---|
| C | -3.24467100 | -1.18671500 | -0.71853600 |
| C | -2.17000600 | -0.65329800 | 0.04891900 |
| C | -2.12049700 | -0.83669700 | 1.43541500 |
| C | -3.18951600 | -1.47832800 | 2.05715500 |
| C | -4.28302600 | -1.95837700 | 1.31276600 |
| C | -4.31114300 | -1.82898700 | -0.07228800 |
| C | -2.91360000 | -0.95387000 | -2.10120600 |
| C | -1.70829500 | -0.31428700 | -2.11268000 |
| H | -1.25364400 | -0.52253900 | 2.00822900 |
| H | -3.16809200 | -1.62628600 | 3.13362900 |
| H | -5.10104800 | -2.45794000 | 1.82512400 |
| H | -5.13693000 | -2.23816300 | -0.64945700 |

| | | | |
|---|---|---|---|
| H | -3.49497800 | -1.24339900 | -2.96718100 |
| H | -1.12677200 | 0.01895500 | -2.96297200 |
| N | -1.23478700 | -0.06726900 | -0.81659800 |
| C | 3.59429200 | -0.63719600 | 0.18313900 |
| C | 3.28946800 | -1.99819900 | 0.31884800 |
| H | 4.11505300 | -2.65853000 | 0.55713600 |
| C | 2.01859100 | -2.59780400 | 0.18049500 |
| O | 0.92830800 | -2.00340900 | -0.09429800 |
| C | 1.89183700 | -4.09692100 | 0.37283400 |
| H | 2.84915200 | -4.57543000 | 0.59388100 |
| H | 1.19060800 | -4.29916000 | 1.19025100 |
| H | 1.46593400 | -4.54289900 | -0.53279900 |
| C | 5.02774100 | -0.18195900 | 0.37482000 |
| H | 5.07114600 | 0.56006400 | 1.18018000 |
| H | 5.70036600 | -1.00900900 | 0.61410600 |
| H | 5.37853400 | 0.31232300 | -0.53833800 |
| Pd | 0.79336400 | 0.05197000 | -0.42690800 |
| O | 2.78296400 | 0.31771600 | -0.09427400 |
| C | 0.43644100 | 2.61875500 | 1.65999200 |
| C | 0.82685000 | 3.15427100 | 0.26010300 |
| C | -1.44409800 | 3.01595900 | 0.13785500 |
| C | -1.11906100 | 2.52943500 | 1.57514800 |
| H | 0.90688600 | 1.65508500 | 1.87091500 |
| H | 0.74926500 | 3.32198100 | 2.44047700 |
| H | -1.51335300 | 1.53391100 | 1.76598600 |
| H | -1.59749400 | 3.21243100 | 2.28534800 |
| C | -0.35099200 | 4.13316600 | -0.01888500 |
| H | -0.31564600 | 4.58193500 | -1.01759200 |
| H | -0.47685300 | 4.93020600 | 0.72526100 |
| C | 0.53580800 | 2.09547900 | -0.82977400 |
| H | 1.09858200 | 2.19123900 | -1.76267800 |
| C | -0.89844800 | 2.09814800 | -0.93487400 |
| H | -1.43730300 | 2.00713100 | -1.86818400 |
| H | 1.83461600 | 3.57059000 | 0.20664000 |
| H | -2.48547400 | 3.30787800 | -0.01089000 |

**int.I-dk**

| | | | |
|---|---|---|---|
| C | 2.45793900 | 2.06913900 | -0.63470600 |
| C | 1.92179700 | 0.96765100 | 0.07149100 |
| C | 1.82053700 | 1.00234100 | 1.46293400 |
| C | 2.38083200 | 2.08488000 | 2.14145900 |
| C | 2.98621500 | 3.14506700 | 1.44908600 |
| C | 3.00713100 | 3.15563700 | 0.05858500 |
| C | 2.22848100 | 1.83449200 | -2.04252600 |

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|---|---|---|---|
| C | 1.58644600 | 0.65344300 | -2.15642900 |
| H | 1.27677400 | 0.24359100 | 2.00976800 |
| H | 2.32010200 | 2.11530000 | 3.22562000 |
| H | 3.40700100 | 3.97903000 | 2.00390100 |
| H | 3.41894100 | 4.00077600 | -0.48635900 |
| H | 2.49359000 | 2.49675800 | -2.85632500 |
| H | 1.25248300 | 0.13249300 | -3.04234000 |
| N | 1.36626900 | 0.03491900 | -0.88327600 |
| C | -3.62092200 | -0.31099400 | 0.29651300 |
| C | -3.70016400 | 1.08759000 | 0.32758000 |
| H | -4.66938200 | 1.50880300 | 0.56863300 |
| C | -2.65612400 | 2.00833000 | 0.07646100 |
| O | -1.45588700 | 1.71997500 | -0.21754400 |
| C | -2.96397000 | 3.49312200 | 0.15715100 |
| H | -4.00446900 | 3.69709700 | 0.42286300 |
| H | -2.30539400 | 3.95967900 | 0.89845500 |
| H | -2.74258700 | 3.96132800 | -0.80883900 |
| C | -4.86795200 | -1.12168800 | 0.59812400 |
| H | -4.67773000 | -1.77860400 | 1.45454200 |
| H | -5.73423200 | -0.49228800 | 0.81616300 |
| H | -5.09945300 | -1.76661900 | -0.25719900 |
| Pd | -0.75827800 | -0.27965400 | -0.40618100 |
| O | -2.59450600 | -1.03699700 | 0.03629100 |
| C | 0.75896400 | -2.65401500 | 1.66532500 |
| C | 0.34038300 | -3.20615200 | 0.27675400 |
| C | 2.44693000 | -2.38610200 | -0.06955400 |
| C | 2.24597200 | -2.23070900 | 1.45025000 |
| H | 0.11694500 | -1.81747400 | 1.96087700 |
| H | 0.67520800 | -3.42436200 | 2.44035900 |
| H | 2.50136500 | -1.24729800 | 1.83496000 |
| H | 2.92059500 | -2.93915600 | 1.94612500 |
| C | 1.69807000 | -3.73915800 | -0.27041600 |
| H | 1.64269500 | -4.07132800 | -1.31351100 |
| H | 2.14193200 | -4.54205400 | 0.33060300 |
| C | 0.11125800 | -2.07227300 | -0.73771000 |
| H | -0.34991200 | -2.45962000 | -1.65488600 |
| C | 1.52533800 | -1.52056700 | -0.97368100 |
| H | 1.87541100 | -1.66931400 | -1.99747000 |
| H | -0.47888200 | -3.92755900 | 0.31950100 |
| H | 3.49608200 | -2.36355000 | -0.37830200 |

**4a**

| | | | |
|---|---|---|---|
| C | -0.25013900 | 0.75234700 | 0.00002100 |
| C | -0.24802700 | -0.67201100 | -0.00005500 |

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|---|---|---|---|
| C | 0.93523300 | -1.41910900 | 0.00002800 |
| C | 2.13635300 | -0.71890000 | 0.00018800 |
| C | 2.15977500 | 0.69168200 | 0.00026300 |
| C | 0.98279600 | 1.42924700 | 0.00018100 |
| C | -1.62641200 | 1.16725200 | -0.00007400 |
| C | -2.39074000 | 0.03025400 | -0.00031500 |
| H | 0.91841700 | -2.50612900 | -0.00002800 |
| H | 3.07354500 | -1.26884600 | 0.00026200 |
| H | 3.11669200 | 1.20665700 | 0.00039200 |
| H | 1.01225000 | 2.51600000 | 0.00024700 |
| H | -1.99888700 | 2.18248100 | -0.00003700 |
| H | -3.46558600 | -0.08722600 | -0.00048700 |
| H | -1.88121200 | -2.03865200 | -0.00023300 |
| N | -1.56689300 | -1.08126700 | -0.00022100 |

**TS2**

| | | | |
|---|---|---|---|
| C | -2.95457700 | -1.87072400 | -0.26240000 |
| C | -3.21873100 | -0.47719900 | -0.46452000 |
| C | -4.47858200 | -0.02711800 | -0.89539800 |
| C | -5.47532400 | -0.97376300 | -1.09588200 |
| C | -5.23952900 | -2.35093300 | -0.87598600 |
| C | -3.99406200 | -2.80143800 | -0.46316800 |
| C | -1.58617900 | -1.96978700 | 0.10999300 |
| C | -1.03909200 | -0.68663600 | 0.15630000 |
| H | -4.67187500 | 1.03040900 | -1.05312100 |
| H | -6.46081600 | -0.64875900 | -1.42268900 |
| H | -6.04742600 | -3.06138400 | -1.03619200 |
| H | -3.81431500 | -3.86222000 | -0.30184800 |
| H | -1.04756700 | -2.86644900 | 0.38671900 |
| H | -0.40440300 | -0.48803700 | 1.23352100 |
| N | -2.07464800 | 0.22074300 | -0.18882100 |
| C | 3.61666000 | 0.23674600 | -1.58545000 |
| C | 3.95255400 | -1.05937400 | -1.16187300 |
| H | 4.98080000 | -1.36830200 | -1.31838000 |
| C | 3.09530500 | -2.00402600 | -0.54926400 |
| O | 1.86891500 | -1.85990600 | -0.28202900 |
| C | 3.68428300 | -3.35290300 | -0.15440900 |
| H | 4.72250200 | -3.47801800 | -0.47746400 |
| H | 3.63607300 | -3.45476000 | 0.93617600 |
| H | 3.07368100 | -4.15652200 | -0.58154400 |
| C | 4.70274100 | 1.08560900 | -2.23443800 |
| H | 4.85188300 | 1.99525200 | -1.64077200 |
| H | 5.65745200 | 0.55862100 | -2.32353300 |
| H | 4.37315000 | 1.40149600 | -3.23133800 |

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|---|---|---|---|
| Pd | 0.80591600 | -0.01272200 | -0.56237400 |
| O | 2.48760800 | 0.82156200 | -1.50009700 |
| C | 0.18247500 | 2.77133900 | 1.33415600 |
| C | 0.15553400 | 3.00027300 | -0.19434400 |
| C | -2.04241300 | 2.74986300 | 0.32705500 |
| C | -1.32269900 | 2.52458200 | 1.67810100 |
| H | 0.82815700 | 1.93944600 | 1.62343600 |
| H | 0.55121300 | 3.67598400 | 1.83841400 |
| H | -1.49062900 | 1.52352200 | 2.08282100 |
| H | -1.68946400 | 3.24401000 | 2.42158800 |
| C | -1.15168500 | 3.82810700 | -0.33423400 |
| H | -1.42887800 | 4.04589800 | -1.37459600 |
| H | -1.13300700 | 4.77064400 | 0.22993100 |
| C | -0.23122300 | 1.70309600 | -0.94472200 |
| H | -0.07200600 | 1.83539200 | -2.02364100 |
| C | -1.76061500 | 1.57064900 | -0.64250900 |
| H | -2.34497600 | 1.73409400 | -1.55859700 |
| H | 1.06517000 | 3.46426700 | -0.58633200 |
| H | -3.10813500 | 2.98922100 | 0.42237700 |
| C | 1.03695800 | -0.43044300 | 3.05723500 |
| O | 1.27536400 | -0.97778600 | 4.31951000 |
| H | 2.20644400 | -0.74776800 | 4.47735600 |
| O | 1.98254500 | 0.14951500 | 2.50216800 |
| O | -0.16111100 | -0.61232800 | 2.66584600 |

**5a**

| | | | |
|---|---|---|---|
| C | -1.75848500 | 0.84891700 | 0.05738400 |
| C | -1.50454800 | -0.54245800 | 0.21549100 |
| C | -2.51342000 | -1.50469500 | 0.09836800 |
| C | -3.80002900 | -1.05405600 | -0.17474200 |
| C | -4.07694800 | 0.32083300 | -0.32787700 |
| C | -3.07165300 | 1.27241000 | -0.21423800 |
| C | -0.50046000 | 1.52042700 | 0.22620000 |
| C | 0.44971600 | 0.56188400 | 0.47493300 |
| H | -2.30156100 | -2.56404000 | 0.21769800 |
| H | -4.60736000 | -1.77483000 | -0.27109700 |
| H | -5.09489800 | 0.63654900 | -0.53936500 |
| H | -3.29409200 | 2.32937200 | -0.33644200 |
| H | -0.32050700 | 2.58618300 | 0.17837500 |
| H | 0.34271500 | -1.55932200 | 0.53715600 |
| N | -0.15809500 | -0.68554000 | 0.48664600 |
| C | 1.90854800 | 0.72468500 | 0.76767000 |
| C | 2.82230800 | -0.07726400 | -0.14267300 |
| H | 2.15271600 | 0.42195800 | 1.79467700 |

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|---|---|---|---|
| H | 2.18474400 | 1.77749400 | 0.66432700 |
| F | 2.64400800 | 0.21668900 | -1.44174800 |
| F | 4.11812000 | 0.14501500 | 0.15797700 |
| F | 2.60617500 | -1.41488900 | 0.00211000 |

**int.II-dk**

| | | | |
|---|---|---|---|
| C | 4.05609500 | 0.24208500 | -0.27794500 |
| O | 2.94187400 | 0.82403800 | -0.44751300 |
| C | 4.27511000 | -1.10334700 | 0.07880600 |
| H | 5.30864600 | -1.41973100 | 0.17842700 |
| C | 3.28430900 | -2.08250400 | 0.32065800 |
| O | 2.03017800 | -1.93486600 | 0.26161700 |
| C | 3.74813100 | -3.48721900 | 0.69829200 |
| H | 4.83784200 | -3.58248800 | 0.74278800 |
| H | 3.32553700 | -3.75775400 | 1.67316000 |
| H | 3.35606200 | -4.20590100 | -0.03109000 |
| C | 5.27737400 | 1.13158500 | -0.49419200 |
| H | 6.22407100 | 0.60505500 | -0.33684700 |
| H | 5.25818300 | 1.53308900 | -1.51456600 |
| H | 5.22793000 | 1.98867800 | 0.18807700 |
| Pd | 1.00694000 | -0.08658200 | -0.23849000 |
| C | -2.82715600 | -1.88988300 | 0.07048600 |
| C | -3.08862000 | -0.52502500 | -0.28884100 |
| C | -4.38709100 | -0.05080300 | -0.49884400 |
| C | -5.44992000 | -0.94356100 | -0.34410700 |
| C | -5.21725000 | -2.28470100 | 0.01628000 |
| C | -3.92250600 | -2.75873900 | 0.22285600 |
| C | -1.40509800 | -2.02296200 | 0.18480900 |
| C | -0.82746600 | -0.79286600 | -0.09567500 |
| H | -4.56721800 | 0.98521000 | -0.77607700 |
| H | -6.46924700 | -0.59660500 | -0.50277100 |
| H | -6.06284700 | -2.96055900 | 0.13430800 |
| H | -3.75816700 | -3.79969100 | 0.49773700 |
| H | -0.85643000 | -2.92100600 | 0.43755700 |
| N | -1.86669800 | 0.10809000 | -0.36822100 |
| C | -1.54611400 | 1.46459700 | -0.75352600 |
| C | -2.04152000 | 2.59388400 | 0.19831200 |
| C | 0.01592500 | 1.63361200 | -0.73228400 |
| H | -1.95685700 | 1.65261500 | -1.75850700 |
| C | -1.03844400 | 3.71336300 | -0.16185600 |
| C | -1.63850400 | 2.26328100 | 1.65392900 |
| H | -3.10299300 | 2.83874600 | 0.07977300 |
| C | 0.21166700 | 2.86439700 | 0.18956000 |
| H | 0.37233200 | 1.88887200 | -1.74044300 |

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|---|---|---|---|
| H | -1.15819200 | 4.61179900 | 0.46073200 |
| H | -1.07891500 | 4.01041900 | -1.21805100 |
| H | -2.15158700 | 2.93622100 | 2.35320900 |
| H | -1.90790500 | 1.23815100 | 1.92326400 |
| C | -0.09364200 | 2.49788100 | 1.66125200 |
| H | 1.18158900 | 3.35207700 | 0.05281600 |
| H | 0.17436700 | 3.32726400 | 2.33156700 |
| H | 0.46333600 | 1.60984000 | 1.97239300 |

**TS3**

| | | | |
|---|---|---|---|
| C | 2.05945000 | 3.07400600 | 0.54123700 |
| O | 1.01830000 | 2.70991800 | -0.09618100 |
| C | 2.62522300 | 2.46037700 | 1.67394800 |
| H | 3.53631500 | 2.90434200 | 2.05987200 |
| C | 2.13533200 | 1.32806200 | 2.36579700 |
| O | 1.09264300 | 0.66158100 | 2.08947600 |
| C | 2.93053400 | 0.81443600 | 3.55574200 |
| H | 3.71535000 | 1.50710400 | 3.87388200 |
| H | 2.25089800 | 0.62089800 | 4.39245600 |
| H | 3.39390200 | -0.14066800 | 3.27996000 |
| C | 2.74249100 | 4.31071200 | -0.02494300 |
| H | 2.02259200 | 5.13667400 | -0.06167900 |
| H | 3.61477600 | 4.62044100 | 0.55776400 |
| H | 3.05527800 | 4.11038000 | -1.05648100 |
| Pd | -0.19325700 | 1.00522500 | 0.36506300 |
| C | -2.70100500 | -2.25545100 | 1.38933000 |
| C | -3.34876800 | -1.63295200 | 0.27358800 |
| C | -4.54208600 | -2.12934000 | -0.26237900 |
| C | -5.10062800 | -3.26452700 | 0.32339000 |
| C | -4.48349100 | -3.88940600 | 1.42531300 |
| C | -3.29623500 | -3.39499900 | 1.95865500 |
| C | -1.51259700 | -1.49776400 | 1.65986300 |
| C | -1.45848900 | -0.46185800 | 0.74383900 |
| H | -5.01828200 | -1.64872500 | -1.11311800 |
| H | -6.02574300 | -3.67321400 | -0.07736200 |
| H | -4.94271700 | -4.77356700 | 1.86285500 |
| H | -2.82703200 | -3.88931700 | 2.80708300 |
| H | -0.78196500 | -1.68745800 | 2.43489200 |
| N | -2.57593700 | -0.54945500 | -0.08747400 |
| C | -2.74191600 | 0.40139800 | -1.16444100 |
| C | -3.98397800 | 1.33831100 | -1.07103600 |
| C | -1.53673100 | 1.40623700 | -1.13253600 |
| H | -2.77496600 | -0.14359900 | -2.11836900 |
| C | -3.48603700 | 2.53992900 | -1.90502800 |

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|---|---|---|---|
| C | -4.07058500 | 1.95096400 | 0.34482900 |
| H | -4.91517100 | 0.87015100 | -1.40724700 |
| C | -2.23180900 | 2.78366100 | -1.02480300 |
| H | -0.96931700 | 1.35639600 | -2.06439000 |
| H | -4.19294100 | 3.38103000 | -1.90814600 |
| H | -3.24254200 | 2.28091800 | -2.94295000 |
| H | -5.03454300 | 2.45683200 | 0.48037100 |
| H | -3.98665800 | 1.18813200 | 1.12377900 |
| C | -2.88576300 | 2.96935400 | 0.36698300 |
| H | -1.58349800 | 3.61280800 | -1.32026700 |
| H | -3.25115000 | 3.99836800 | 0.48458900 |
| H | -2.17954100 | 2.77359200 | 1.18030700 |
| C | 1.09629200 | -0.74976500 | -2.07339700 |
| C | 1.50668900 | -0.58928400 | -0.62636600 |
| H | 2.12478500 | 0.24842700 | -0.35909500 |
| H | 1.11749700 | -1.27113300 | 0.10810400 |
| F | -0.17789400 | -1.20136300 | -2.17563900 |
| F | 1.16374800 | 0.44180600 | -2.72234100 |
| F | 1.84132900 | -1.60781900 | -2.79498900 |
| I | 3.87148100 | -1.98058800 | -0.32325500 |

**int.IV-dk**

| | | | |
|---|---|---|---|
| C | -3.99639600 | 0.43020500 | -0.28578900 |
| O | -2.89656100 | 0.87313000 | 0.19763800 |
| C | -4.16173500 | -0.69439600 | -1.11162500 |
| H | -5.17455600 | -0.91759400 | -1.42563900 |
| C | -3.15075100 | -1.55371700 | -1.59173100 |
| O | -1.90402700 | -1.47528800 | -1.33928300 |
| C | -3.54427600 | -2.69754000 | -2.50735800 |
| H | -4.62106700 | -2.74589800 | -2.68726700 |
| H | -3.02516200 | -2.58593100 | -3.46617200 |
| H | -3.20861900 | -3.64457900 | -2.07006400 |
| C | -5.22010100 | 1.23973100 | 0.09772800 |
| H | -6.14317000 | 0.83601000 | -0.32518700 |
| H | -5.30869600 | 1.27086100 | 1.18969400 |
| H | -5.09210600 | 2.27358700 | -0.24304300 |
| Pd | -0.96538800 | 0.02777500 | -0.10048400 |
| C | 2.86340200 | -1.39475500 | -1.10678900 |
| C | 3.10942800 | -0.22593400 | -0.32099500 |
| C | 4.40533900 | 0.24027900 | -0.06707100 |
| C | 5.46679100 | -0.48619500 | -0.59580200 |
| C | 5.24757600 | -1.64661300 | -1.36886600 |
| C | 3.96235500 | -2.10277400 | -1.62914000 |
| C | 1.44182800 | -1.57471700 | -1.17233100 |

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|---|---|---|---|
| C | 0.87959200 | -0.53345500 | -0.46336100 |
| H | 4.57939600 | 1.13024200 | 0.53088900 |
| H | 6.48464200 | -0.15507400 | -0.40786500 |
| H | 6.10165100 | -2.18875200 | -1.76591100 |
| H | 3.80308900 | -2.99634400 | -2.22747600 |
| H | 0.90071700 | -2.37233900 | -1.66147300 |
| N | 1.88102700 | 0.27157900 | 0.06788800 |
| C | 1.53560600 | 1.50701600 | 0.73808000 |
| C | 1.90372600 | 2.82139500 | -0.01555000 |
| C | -0.02609200 | 1.60006100 | 0.83863300 |
| H | 1.98819900 | 1.51517900 | 1.73693700 |
| C | 0.84468300 | 3.78216100 | 0.56986100 |
| C | 1.45772300 | 2.72331500 | -1.49189000 |
| H | 2.94802300 | 3.11828500 | 0.11319300 |
| C | -0.36642200 | 2.92060000 | 0.12454400 |
| H | -0.37182800 | 1.60548200 | 1.87239200 |
| H | 0.85909100 | 4.77397100 | 0.10214700 |
| H | 0.91292800 | 3.90531000 | 1.65703400 |
| H | 1.86288800 | 3.56481700 | -2.06391000 |
| H | 1.80678800 | 1.80488100 | -1.97079400 |
| C | -0.09973100 | 2.80371700 | -1.40017700 |
| H | -1.35885000 | 3.30035600 | 0.37447500 |
| H | -0.48963400 | 3.68723400 | -1.91851600 |
| H | -0.59130200 | 1.93482600 | -1.86029900 |
| C | -0.03960900 | -1.39858800 | 2.54765500 |
| C | -1.16672000 | -1.10006400 | 1.59128800 |
| H | -1.95304400 | -0.55980300 | 2.12058300 |
| H | -1.54133600 | -2.03931100 | 1.18137300 |
| F | 0.53490500 | -0.28928200 | 3.07030100 |
| F | -0.56058800 | -2.09273800 | 3.59592900 |
| F | 0.93679900 | -2.15522700 | 2.02479500 |

**TS4**

| | | | |
|---|---|---|---|
| C | -3.65879500 | 1.23366100 | -0.46807300 |
| O | -2.54722500 | 1.50452800 | 0.11038000 |
| C | -3.96454700 | 0.09634500 | -1.22938900 |
| H | -4.96690400 | 0.04282100 | -1.63787900 |
| C | -3.09946400 | -0.97636100 | -1.53761500 |
| O | -1.89189800 | -1.10826200 | -1.16374300 |
| C | -3.62433200 | -2.10643900 | -2.40384100 |
| H | -4.65562200 | -1.94780800 | -2.72895500 |
| H | -2.98189900 | -2.21637700 | -3.28469400 |
| H | -3.56528200 | -3.04573600 | -1.84223100 |
| C | -4.72558700 | 2.29584500 | -0.28047600 |

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|---|---|---|---|
| H | -5.66321900 | 2.04460400 | -0.78230000 |
| H | -4.91775000 | 2.43304000 | 0.78982400 |
| H | -4.35745700 | 3.25321900 | -0.66681200 |
| Pd | -0.85851300 | 0.26985000 | 0.10017800 |
| C | 2.81788500 | -1.50318000 | -0.88673400 |
| C | 3.16267600 | -0.36757800 | -0.08381700 |
| C | 4.49416200 | 0.04967400 | 0.06488000 |
| C | 5.47666900 | -0.68741000 | -0.58334700 |
| C | 5.15659800 | -1.81301700 | -1.37736800 |
| C | 3.84306600 | -2.22273900 | -1.53589000 |
| C | 1.40372800 | -1.65106900 | -0.82626100 |
| C | 0.91965100 | -0.62110900 | -0.02632400 |
| H | 4.75366100 | 0.90749100 | 0.67632500 |
| H | 6.51730500 | -0.39436400 | -0.47406300 |
| H | 5.95650800 | -2.36057200 | -1.86779300 |
| H | 3.59918900 | -3.08676200 | -2.14822600 |
| H | 0.80195800 | -2.42507300 | -1.27797900 |
| N | 1.99413800 | 0.15162600 | 0.42945700 |
| C | 1.74739800 | 1.40763300 | 1.13004600 |
| C | 2.34671200 | 2.68969600 | 0.48125100 |
| C | 0.20557100 | 1.70718100 | 1.11901600 |
| H | 2.12830000 | 1.31847300 | 2.15724700 |
| C | 1.40322400 | 3.75713400 | 1.08085800 |
| C | 1.98111100 | 2.75085700 | -1.02015000 |
| H | 3.41201000 | 2.82606700 | 0.68580900 |
| C | 0.11404600 | 3.11799900 | 0.50440400 |
| H | -0.20623800 | 1.71159200 | 2.13513400 |
| H | 1.59955800 | 4.76368400 | 0.69243200 |
| H | 1.42262000 | 3.79391700 | 2.17664600 |
| H | 2.55899800 | 3.54053400 | -1.51250800 |
| H | 2.20364800 | 1.81610600 | -1.54175600 |
| C | 0.45551800 | 3.08472700 | -1.00563500 |
| H | -0.82767100 | 3.61932900 | 0.73347500 |
| H | 0.25918900 | 4.06501400 | -1.45581500 |
| H | -0.14231500 | 2.34982100 | -1.55313400 |
| C | -0.99024000 | -2.44408700 | 1.57537000 |
| C | -0.07690800 | -1.23768700 | 1.61886600 |
| H | 0.90661800 | -1.57358100 | 1.93717800 |
| H | -0.45356600 | -0.55364300 | 2.38007800 |
| F | -0.72830900 | -3.29811600 | 0.57195000 |
| F | -0.82658300 | -3.13364900 | 2.73665600 |
| F | -2.29676000 | -2.11121900 | 1.50960100 |

**int.VII**

| | | | |
|---|---|---|---|
| C | -2.98441500 | 2.03375500 | -0.59787200 |
| O | -1.87078400 | 1.91528900 | 0.02511200 |
| C | -3.57790700 | 1.11489500 | -1.47387900 |
| H | -4.52791400 | 1.40398300 | -1.90786400 |
| C | -3.06193300 | -0.14128600 | -1.85718400 |
| O | -1.97130300 | -0.66202400 | -1.46433500 |
| C | -3.85835000 | -0.98277900 | -2.83861800 |
| H | -4.78748900 | -0.50046500 | -3.15274200 |
| H | -3.24445500 | -1.18744200 | -3.72326200 |
| H | -4.09398300 | -1.94914800 | -2.37839600 |
| C | -3.69792100 | 3.34456000 | -0.32166600 |
| H | -4.63385000 | 3.43696700 | -0.87800700 |
| H | -3.90969700 | 3.42440500 | 0.75076900 |
| H | -3.03968700 | 4.18038700 | -0.58408700 |
| Pd | -0.64466400 | 0.25255900 | -0.03985000 |
| C | 1.80429800 | -1.43141000 | -1.37151700 |
| C | 2.67826100 | -0.80083000 | -0.45159700 |
| C | 3.99061200 | -0.47883600 | -0.81817900 |
| C | 4.39945700 | -0.78648000 | -2.11308200 |
| C | 3.53190300 | -1.40060700 | -3.03730600 |
| C | 2.23094600 | -1.72850400 | -2.67376100 |
| C | 0.58558900 | -1.72193000 | -0.65580300 |
| C | 0.76262600 | -1.31384400 | 0.67092100 |
| H | 4.67288800 | -0.01571600 | -0.11338800 |
| H | 5.41860800 | -0.55754600 | -2.41281300 |
| H | 3.89054400 | -1.63128200 | -4.03616900 |
| H | 1.55964600 | -2.21758600 | -3.37429700 |
| H | -0.21309200 | -2.35670700 | -1.01155300 |
| N | 2.03796700 | -0.66925700 | 0.78455400 |
| C | 1.93690500 | 0.58860400 | 1.57528000 |
| C | 2.83824000 | 1.81281300 | 1.27210800 |
| C | 0.48925900 | 1.18750600 | 1.42405600 |
| H | 2.12541500 | 0.31365300 | 2.62088000 |
| C | 2.05252400 | 2.86024500 | 2.10449000 |
| C | 2.65485400 | 2.39770900 | -0.15698200 |
| H | 3.88394400 | 1.66773800 | 1.56028700 |
| C | 0.73799400 | 2.70594100 | 1.29171300 |
| H | -0.11117600 | 0.98578700 | 2.32156800 |
| H | 2.48637300 | 3.86487600 | 2.03131000 |
| H | 1.95673300 | 2.59678800 | 3.16444800 |
| H | 3.43886100 | 3.14359400 | -0.33351200 |
| H | 2.74299800 | 1.65643400 | -0.94897400 |
| C | 1.24162100 | 3.05397400 | -0.12376800 |

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|---|---|---|---|
| H | -0.10919200 | 3.31032100 | 1.61946100 |
| H | 1.30466600 | 4.14185400 | -0.25022500 |
| H | 0.57714700 | 2.66605700 | -0.89918100 |
| C | -1.15638800 | -2.54280200 | 1.92830300 |
| C | 0.24420100 | -1.95754700 | 1.94403300 |
| H | 0.91802900 | -2.78610900 | 2.19999000 |
| H | 0.28030900 | -1.25266200 | 2.77880300 |
| F | -1.34919600 | -3.39987100 | 0.90078900 |
| F | -1.36026300 | -3.23635700 | 3.07184800 |
| F | -2.12547300 | -1.60556000 | 1.86000600 |

**TS5**

| | | | |
|---|---|---|---|
| C | -3.29261400 | -0.23092000 | 0.73840700 |
| C | -2.04079200 | 0.41803300 | 0.92067100 |
| C | -1.77273200 | 1.13888500 | 2.08923300 |
| C | -2.79246600 | 1.27876400 | 3.02837500 |
| C | -4.05443800 | 0.68968100 | 2.82721200 |
| C | -4.30727500 | -0.07767300 | 1.69474800 |
| C | -3.17187400 | -1.00649900 | -0.46566300 |
| C | -1.90906900 | -0.81240700 | -0.95336900 |
| H | -0.78223200 | 1.53760700 | 2.28256600 |
| H | -2.60078300 | 1.83470100 | 3.94221800 |
| H | -4.82864000 | 0.81299300 | 3.57978100 |
| H | -5.26668400 | -0.57172900 | 1.56267600 |
| H | -3.91764600 | -1.66661300 | -0.89026800 |
| N | -1.19598200 | 0.11053300 | -0.15807000 |
| C | 3.67824700 | -0.32743700 | 0.70976300 |
| C | 3.30482300 | -1.22773500 | 1.71565500 |
| H | 4.10946300 | -1.69264800 | 2.27303600 |
| C | 1.98918500 | -1.58716500 | 2.08393900 |
| O | 0.91436000 | -1.15526500 | 1.56032800 |
| C | 1.79017300 | -2.58158900 | 3.21142700 |
| H | 2.73373800 | -2.91640000 | 3.64943200 |
| H | 1.17059200 | -2.12639100 | 3.99204500 |
| H | 1.24132800 | -3.45050300 | 2.83131700 |
| C | 5.15126000 | -0.05878200 | 0.47247100 |
| H | 5.35277100 | 1.01130500 | 0.59684400 |
| H | 5.79368500 | -0.62464900 | 1.15132000 |
| H | 5.40697500 | -0.31731300 | -0.56143000 |
| Pd | 0.87618100 | 0.17498400 | -0.04496500 |
| O | 2.90251500 | 0.33197100 | -0.07305300 |
| C | 1.10278700 | 3.48358500 | -0.12160200 |
| C | 1.23325900 | 2.93920200 | -1.56419600 |
| C | -1.02218200 | 3.13054900 | -1.29543000 |

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|---|---|---|---|
| C | -0.44083300 | 3.62073900 | 0.05647700 |
| H | 1.55766400 | 2.80895200 | 0.60751100 |
| H | 1.59862600 | 4.45716300 | -0.03282600 |
| H | -0.83654900 | 3.06161400 | 0.90043100 |
| H | -0.73503000 | 4.66698100 | 0.19365400 |
| C | 0.07186800 | 3.69712400 | -2.27205900 |
| H | -0.06831500 | 3.40011100 | -3.31723200 |
| H | 0.13186200 | 4.79177300 | -2.21895200 |
| C | 0.68438200 | 1.49472800 | -1.65973100 |
| H | 1.06725100 | 0.90096700 | -2.49509800 |
| C | -0.74789800 | 1.66916900 | -1.58973600 |
| H | -1.45488800 | 1.14908700 | -2.22291500 |
| H | 2.22942000 | 3.05403800 | -1.99578000 |
| H | -2.05577900 | 3.43347000 | -1.47346200 |
| C | -1.29385700 | -1.47972700 | -2.14930400 |
| C | -0.81936200 | -2.90272800 | -1.88786000 |
| H | -0.42531400 | -0.93077800 | -2.52140100 |
| H | -2.02039800 | -1.55065100 | -2.96696300 |
| F | -1.83272100 | -3.70752400 | -1.50688600 |
| F | -0.28871500 | -3.42930800 | -3.01775800 |
| F | 0.13120200 | -2.96500500 | -0.93384400 |

**int.VIII**

| | | | |
|---|---|---|---|
| C | -3.51582600 | -1.23860200 | 0.01248500 |
| C | -2.17726200 | -1.32081800 | -0.48180600 |
| C | -1.88958000 | -2.01357500 | -1.67030300 |
| C | -2.93342400 | -2.65151300 | -2.33206200 |
| C | -4.25168600 | -2.60669100 | -1.83187400 |
| C | -4.54834000 | -1.90618700 | -0.66962700 |
| C | -3.45025700 | -0.42417900 | 1.18269300 |
| C | -2.12918900 | -0.06007900 | 1.35351300 |
| H | -0.88233500 | -2.02999600 | -2.07995600 |
| H | -2.72992700 | -3.19028400 | -3.25410900 |
| H | -5.04402200 | -3.12088700 | -2.36982300 |
| H | -5.56843200 | -1.86678000 | -0.29401200 |
| H | -4.26660300 | -0.16000600 | 1.84368100 |
| N | -1.33121500 | -0.64123700 | 0.37635200 |
| C | 2.41606800 | 1.74117100 | -1.64893300 |
| C | 1.39075900 | 2.57562800 | -2.11018500 |
| H | 1.67999900 | 3.44258500 | -2.69139600 |
| C | 0.01682900 | 2.37506800 | -1.89550700 |
| O | -0.51635500 | 1.41130900 | -1.25076500 |
| C | -0.98444900 | 3.36166200 | -2.45508900 |
| H | -0.50640200 | 4.16724900 | -3.01734800 |

| | | | |
|---|---|---|---|
| H | -1.69225400 | 2.83392000 | -3.10335300 |
| H | -1.56085300 | 3.78675700 | -1.62597300 |
| C | 3.85246400 | 2.07537600 | -1.99569400 |
| H | 4.30181000 | 1.23870400 | -2.54255000 |
| H | 3.93359900 | 2.98143200 | -2.60044100 |
| H | 4.43030700 | 2.20757100 | -1.07391700 |
| Pd | 0.49838700 | -0.04117200 | -0.24164500 |
| O | 2.28509100 | 0.68140800 | -0.93852900 |
| C | 3.78697000 | -1.12824900 | 0.96559500 |
| C | 2.74381400 | -1.72045800 | 1.95659000 |
| C | 2.46769500 | -2.99411500 | 0.10725300 |
| C | 3.59089100 | -2.00021100 | -0.31262800 |
| H | 3.62627900 | -0.06860800 | 0.77081700 |
| H | 4.79121200 | -1.25366800 | 1.38548700 |
| H | 3.31672000 | -1.40202700 | -1.18154000 |
| H | 4.49753500 | -2.56507100 | -0.55610100 |
| C | 2.85807300 | -3.23326500 | 1.59780100 |
| H | 2.14396000 | -3.86378600 | 2.13779600 |
| H | 3.86996600 | -3.63761100 | 1.72479200 |
| C | 1.31207500 | -1.48702300 | 1.46565600 |
| H | 0.52298200 | -1.11263400 | 2.10449700 |
| C | 1.14112900 | -2.26888500 | 0.34490400 |
| H | 0.19853800 | -2.60719500 | -0.06862600 |
| H | 2.90599300 | -1.44040200 | 2.99992900 |
| H | 2.38197800 | -3.87327900 | -0.53510600 |
| C | -1.61901800 | 0.77524900 | 2.49317200 |
| C | -1.14776700 | 2.18843700 | 2.17101600 |
| H | -0.79619900 | 0.29783600 | 3.04044900 |
| H | -2.43847200 | 0.89717200 | 3.20808100 |
| F | -1.97022000 | 2.83747100 | 1.32861800 |
| F | -1.06595900 | 2.92077000 | 3.30788500 |
| F | 0.09702400 | 2.21369300 | 1.61821400 |

**int.IX**

| | | | |
|---|---|---|---|
| C | -2.21115600 | 2.39775200 | 0.67319000 |
| C | -1.26482800 | 1.87209200 | -0.26433500 |
| C | -1.02836900 | 2.52114500 | -1.48990100 |
| C | -1.76269300 | 3.66574900 | -1.78729300 |
| C | -2.71798700 | 4.17466100 | -0.88153700 |
| C | -2.94047300 | 3.55396900 | 0.34136800 |
| C | -2.16918300 | 1.52406100 | 1.79959200 |
| C | -1.24782700 | 0.53428100 | 1.51141100 |
| H | -0.26028800 | 2.15983800 | -2.17087600 |
| H | -1.58747000 | 4.18420000 | -2.72690200 |

| | | | |
|---|---|---|---|
| H | -3.27644500 | 5.06997200 | -1.14264400 |
| H | -3.66957200 | 3.95980100 | 1.03945700 |
| H | -2.76173100 | 1.58949200 | 2.70364900 |
| N | -0.71670700 | 0.71539900 | 0.24634100 |
| C | 3.68158800 | -0.69411800 | -1.34273900 |
| C | 4.12090400 | 0.36369200 | -0.53883500 |
| H | 5.18944600 | 0.53761100 | -0.50285400 |
| C | 3.31271800 | 1.22936400 | 0.22657800 |
| O | 2.04217500 | 1.20272900 | 0.32339600 |
| C | 3.96773700 | 2.32588200 | 1.03991700 |
| H | 5.05307200 | 2.34689300 | 0.91676200 |
| H | 3.54867000 | 3.29417100 | 0.74579500 |
| H | 3.72552000 | 2.17827900 | 2.09816600 |
| C | 4.69791200 | -1.51782400 | -2.10515800 |
| H | 4.45791200 | -1.49874200 | -3.17417400 |
| H | 5.71866000 | -1.15700200 | -1.96041200 |
| H | 4.63863700 | -2.56249900 | -1.77873400 |
| Pd | 0.86476400 | -0.18946300 | -0.61200800 |
| O | 2.46640800 | -1.07252200 | -1.52143300 |
| C | -0.93578800 | -0.64023800 | 2.39178100 |
| C | 0.44412500 | -0.68601700 | 3.02999600 |
| H | -1.06830800 | -1.59030300 | 1.86232300 |
| H | -1.64502800 | -0.63563500 | 3.22520000 |
| F | 0.82711400 | 0.49434300 | 3.54769500 |
| F | 0.46128400 | -1.59603200 | 4.03529300 |
| F | 1.41482700 | -1.07519200 | 2.15691100 |
| C | -1.53737500 | -2.31192200 | -0.92780300 |
| C | -2.46840300 | -1.37212600 | -1.43095100 |
| C | -3.80549000 | -1.36155100 | -1.02859100 |
| C | -4.20730900 | -2.34744500 | -0.13179900 |
| C | -3.30563000 | -3.31651000 | 0.35021400 |
| C | -1.96915500 | -3.30501300 | -0.03743400 |
| C | -0.25133900 | -1.98745900 | -1.51726900 |
| C | -0.48109800 | -0.90684500 | -2.39563100 |
| H | -4.50447100 | -0.61946400 | -1.40224400 |
| H | -5.24202900 | -2.37370900 | 0.19787200 |
| H | -3.66054800 | -4.07881400 | 1.03765300 |
| H | -1.27240800 | -4.04726600 | 0.34338700 |
| H | 0.60422500 | -2.64768200 | -1.56629400 |
| H | 0.15838800 | -0.52450100 | -3.17959900 |
| H | -2.14712800 | 0.34990700 | -2.62784200 |
| N | -1.81203900 | -0.56717600 | -2.35616100 |

**TS6**

| | | | |
|---|---|---|---|
| C | -1.03734900 | -0.32627200 | 1.68904100 |
| C | -1.86566600 | -1.34477800 | 1.16845000 |
| C | -2.05209500 | -2.55335100 | 1.83591900 |
| C | -1.39720100 | -2.72533400 | 3.05628600 |
| C | -0.57670900 | -1.71651800 | 3.58873600 |
| C | -0.38700700 | -0.51071700 | 2.91313900 |
| C | -1.08335300 | 0.77331800 | 0.71755600 |
| C | -2.06453700 | 0.35336800 | -0.23800800 |
| H | -2.70152700 | -3.32340600 | 1.43085500 |
| H | -1.53125000 | -3.65141200 | 3.60843800 |
| H | -0.08777500 | -1.87775500 | 4.54567500 |
| H | 0.24827500 | 0.26847200 | 3.32403700 |
| H | -0.97484800 | 1.81336500 | 1.00383100 |
| N | -2.45982400 | -0.91542800 | -0.04280900 |
| C | 3.73615100 | 1.54695400 | -0.54970800 |
| C | 3.57669600 | 2.47025800 | 0.49600200 |
| H | 4.44414500 | 3.06358000 | 0.75872300 |
| C | 2.40588200 | 2.70021300 | 1.23718900 |
| O | 1.27901300 | 2.11541500 | 1.09462100 |
| C | 2.42727600 | 3.74412600 | 2.33702300 |
| H | 1.66802700 | 4.50661800 | 2.12963100 |
| H | 2.16074700 | 3.27455800 | 3.29057800 |
| H | 3.40212800 | 4.22734200 | 2.43656700 |
| C | 5.08671900 | 1.43753200 | -1.23121900 |
| H | 4.97195900 | 1.63967100 | -2.30211500 |
| H | 5.82315400 | 2.12821900 | -0.81375600 |
| H | 5.46168500 | 0.41239000 | -1.13439900 |
| Pd | 0.88442500 | 0.63644400 | -0.32739800 |
| O | 2.85024100 | 0.75437600 | -1.01975400 |
| C | -2.67225500 | 1.18651400 | -1.33035900 |
| C | -3.70054700 | 2.17602400 | -0.79702800 |
| H | -3.18993900 | 0.55111100 | -2.05522900 |
| H | -1.91743100 | 1.77836100 | -1.85590200 |
| F | -3.13465100 | 3.07668900 | 0.03792900 |
| F | -4.25557400 | 2.86642800 | -1.81683300 |
| F | -4.69376100 | 1.56670800 | -0.12532900 |
| C | 1.09233200 | -2.22961400 | -1.27651100 |
| C | -0.17349200 | -2.85675300 | -1.22505400 |
| C | -0.33929100 | -4.12642000 | -0.67608800 |
| C | 0.79466100 | -4.77048600 | -0.17728400 |
| C | 2.05840100 | -4.15969100 | -0.22812000 |
| C | 2.22007600 | -2.88671900 | -0.77746600 |
| C | 0.87739600 | -0.92612400 | -1.92045200 |

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|---|---|---|---|
| C | -0.49841600 | -0.96151700 | -2.29961900 |
| H | -1.31412500 | -4.60449700 | -0.65500000 |
| H | 0.69914800 | -5.76506900 | 0.24977300 |
| H | 2.92310000 | -4.69030400 | 0.16112400 |
| H | 3.19780200 | -2.41485400 | -0.81810500 |
| H | 1.63545900 | -0.43911400 | -2.52452200 |
| H | -1.02013600 | -0.19971200 | -2.86480800 |
| H | -2.13784300 | -1.64936500 | -1.04606200 |
| N | -1.15281700 | -2.03249300 | -1.83496700 |

**int.XII**

| | | | |
|---|---|---|---|
| C | -2.83471800 | 1.02837300 | -0.22274500 |
| C | -3.28965700 | -0.28848500 | -0.39075300 |
| H | -4.33459200 | -0.41218400 | -0.64880900 |
| C | -2.52900400 | -1.46458100 | -0.25019000 |
| O | -1.29060500 | -1.53923200 | 0.04766000 |
| C | -3.20335700 | -2.80563800 | -0.46375400 |
| H | -4.26524800 | -2.70794900 | -0.70173700 |
| H | -2.70054400 | -3.33851100 | -1.27873700 |
| H | -3.09144000 | -3.41668200 | 0.43885000 |
| C | -3.81069200 | 2.17435700 | -0.40510000 |
| H | -3.44942900 | 2.83659000 | -1.19983900 |
| H | -4.81659900 | 1.82939200 | -0.65560600 |
| H | -3.85257500 | 2.76714400 | 0.51551000 |
| Pd | -0.09351200 | 0.11310600 | 0.38398900 |
| O | -1.64925600 | 1.40657500 | 0.07969200 |
| C | 2.12294400 | 0.31863300 | 0.62696900 |
| C | 2.80462500 | 0.49358500 | -0.62912500 |
| C | 3.36964500 | -0.58628900 | -1.27129400 |
| C | 3.20657400 | -1.87670200 | -0.70306500 |
| C | 2.48242500 | -2.07284500 | 0.46021100 |
| C | 1.89821600 | -0.97336700 | 1.15599100 |
| C | 1.42775200 | 1.55655700 | 0.87654700 |
| C | 1.90148600 | 2.41487600 | -0.23024800 |
| H | 3.89216100 | -0.45498500 | -2.21424900 |
| H | 3.65018000 | -2.73161400 | -1.20569000 |
| H | 2.37757200 | -3.07212600 | 0.87186200 |
| H | 1.49717900 | -1.12120100 | 2.15570500 |
| H | 1.15234700 | 1.95863300 | 1.84764900 |
| H | 1.63864900 | 3.46230200 | -0.35117600 |
| N | 2.69218900 | 1.82124700 | -1.08238600 |

**int.X**

| | | | |
|---|---|---|---|
| C | 3.62847200 | -1.68374900 | -0.76066200 |
| C | 3.71592200 | -0.67369000 | 0.24562600 |

| | | | |
|---|---|---|---|
| C | 4.90714800 | -0.40649800 | 0.93023400 |
| C | 6.02929100 | -1.15967600 | 0.59616100 |
| C | 5.96778500 | -2.15539300 | -0.39990800 |
| C | 4.78320600 | -2.42131600 | -1.07746500 |
| C | 2.27179300 | -1.69503200 | -1.23642400 |
| C | 1.58471600 | -0.72660900 | -0.53005400 |
| H | 4.95808600 | 0.36081600 | 1.69789900 |
| H | 6.96841500 | -0.97549000 | 1.11139100 |
| H | 6.86279100 | -2.72417700 | -0.63892700 |
| H | 4.74668800 | -3.19431600 | -1.84151400 |
| H | 1.86508900 | -2.33887600 | -2.00541700 |
| N | 2.46226100 | -0.10352900 | 0.35437000 |
| C | 1.95899200 | 0.91190400 | 1.24221700 |
| C | 2.52568400 | 2.35089500 | 1.07205900 |
| C | 0.43077000 | 1.10713200 | 0.94617700 |
| H | 2.10554000 | 0.59320800 | 2.28485300 |
| C | 1.35408400 | 3.16937300 | 1.65834000 |
| C | 2.48958000 | 2.75744200 | -0.41775800 |
| H | 3.49889600 | 2.49474800 | 1.54966500 |
| C | 0.30253100 | 2.61314600 | 0.65656100 |
| H | -0.18423400 | 0.80587700 | 1.80269700 |
| H | 1.49573900 | 4.25278300 | 1.56667800 |
| H | 1.13084700 | 2.93161600 | 2.70530400 |
| H | 3.06045500 | 3.67934300 | -0.57334900 |
| H | 2.92551200 | 1.98766100 | -1.06012000 |
| C | 0.96771900 | 2.97837100 | -0.69338900 |
| H | -0.71647600 | 2.99486900 | 0.77027000 |
| H | 0.75798500 | 4.02522400 | -0.94449600 |
| H | 0.59770100 | 2.35187200 | -1.51057400 |
| Pd | -0.29597300 | -0.15703500 | -0.49556300 |
| I | -2.98964700 | 0.55333500 | -0.93625700 |
| C | -4.24619900 | -0.75415000 | 0.31774200 |
| C | -3.44931900 | -1.65187300 | 1.24370200 |
| H | -4.83573500 | -1.35661100 | -0.37102400 |
| H | -4.88401700 | -0.08930200 | 0.89763500 |
| F | -2.69387600 | -0.94918700 | 2.10713200 |
| F | -2.64367400 | -2.49026200 | 0.56750900 |
| F | -4.31312900 | -2.39825900 | 1.96280400 |

**TS7**

| | | | |
|---|---|---|---|
| C | 3.38987600 | -1.43149600 | -1.03229900 |
| C | 3.48503800 | -0.51911100 | 0.06287900 |
| C | 4.68850000 | -0.29132800 | 0.73976700 |
| C | 5.81344800 | -0.98907500 | 0.30988500 |

| | | | |
|---|---|---|---|
| C | 5.74403700 | -1.89035300 | -0.77283600 |
| C | 4.54870800 | -2.11483900 | -1.44474300 |
| C | 2.02322700 | -1.42407700 | -1.47439800 |
| C | 1.33706800 | -0.53559700 | -0.66508700 |
| H | 4.74603100 | 0.40272000 | 1.57363400 |
| H | 6.76216200 | -0.83553800 | 0.81719500 |
| H | 6.64251700 | -2.41684300 | -1.08387600 |
| H | 4.50617700 | -2.81232400 | -2.27776300 |
| H | 1.60934900 | -2.00125800 | -2.29128700 |
| N | 2.22414000 | 0.01145100 | 0.25541300 |
| C | 1.72820900 | 0.95413700 | 1.22259000 |
| C | 2.25152900 | 2.41669300 | 1.12928000 |
| C | 0.19125600 | 1.12790300 | 0.97814500 |
| H | 1.90914100 | 0.57285200 | 2.23799400 |
| C | 1.07119100 | 3.16000600 | 1.79336300 |
| C | 2.16696900 | 2.91430000 | -0.33090900 |
| H | 3.23140000 | 2.55828300 | 1.59332800 |
| C | 0.00920000 | 2.63929300 | 0.78047700 |
| H | -0.40547300 | 0.74079600 | 1.80831000 |
| H | 1.17591500 | 4.25082900 | 1.76612000 |
| H | 0.88014100 | 2.85074300 | 2.82764000 |
| H | 2.70944600 | 3.85934800 | -0.44094500 |
| H | 2.60700400 | 2.19959800 | -1.03164800 |
| C | 0.63364600 | 3.11033600 | -0.55658000 |
| H | -1.01717200 | 2.97957900 | 0.94034400 |
| H | 0.38874300 | 4.16503200 | -0.72829800 |
| H | 0.25678000 | 2.53819000 | -1.40992900 |
| Pd | -0.57154500 | -0.01711100 | -0.56737900 |
| I | -3.23906300 | 0.26631300 | -0.98899400 |
| C | -2.33893000 | -1.81979300 | 0.14443500 |
| C | -2.14106900 | -1.79054500 | 1.64609900 |
| H | -1.53498400 | -2.33609200 | -0.37639900 |
| H | -3.29734000 | -2.26783800 | -0.09241600 |
| F | -2.71506600 | -2.89962400 | 2.16992300 |
| F | -0.84226300 | -1.81460500 | 2.00068100 |
| F | -2.70809600 | -0.72515200 | 2.24226500 |

**int.XI**

| | | | |
|---|---|---|---|
| C | 3.11308900 | -0.55608400 | -1.47294300 |
| C | 3.17232300 | 0.11649500 | -0.21429600 |
| C | 4.38439800 | 0.52162400 | 0.35698400 |
| C | 5.55161800 | 0.23143400 | -0.34081800 |
| C | 5.51739700 | -0.43851100 | -1.58283800 |
| C | 4.31472200 | -0.83128400 | -2.15325100 |

| | | | |
|---|---|---|---|
| C | 1.73017300 | -0.81195800 | -1.75882500 |
| C | 1.00715200 | -0.28710900 | -0.70576100 |
| H | 4.41818700 | 1.03155900 | 1.31527900 |
| H | 6.50950900 | 0.52346300 | 0.08058400 |
| H | 6.45067900 | -0.64831600 | -2.09789600 |
| H | 4.29684500 | -1.34506000 | -3.11075500 |
| H | 1.33131800 | -1.33627500 | -2.61676900 |
| N | 1.87159700 | 0.25511900 | 0.23439900 |
| C | 1.32885900 | 1.00548100 | 1.33894500 |
| C | 1.55614200 | 2.54663100 | 1.32126000 |
| C | -0.23220200 | 0.90719900 | 1.27750100 |
| H | 1.68956900 | 0.58704500 | 2.28687100 |
| C | 0.32916600 | 3.00680400 | 2.13900300 |
| C | 1.23628700 | 3.11167400 | -0.08025200 |
| H | 2.53281000 | 2.84332500 | 1.71138700 |
| C | -0.71719900 | 2.35201600 | 1.18751600 |
| H | -0.66887600 | 0.34570600 | 2.10189100 |
| H | 0.21824600 | 4.09608600 | 2.18082300 |
| H | 0.30120400 | 2.61134500 | 3.16072700 |
| H | 1.55496200 | 4.15709900 | -0.14495000 |
| H | 1.74970200 | 2.56525700 | -0.87570800 |
| C | -0.31792000 | 2.99096300 | -0.17049800 |
| H | -1.76868000 | 2.47491300 | 1.45042700 |
| H | -0.79781500 | 3.97039900 | -0.26810400 |
| H | -0.64862500 | 2.39725100 | -1.03227100 |
| Pd | -0.93697600 | -0.16539500 | -0.36284600 |
| I | -3.58728500 | 0.13229400 | -0.74029300 |
| C | -1.07833400 | -2.02007700 | 0.50379600 |
| C | 0.04596800 | -2.60738300 | 1.32227500 |
| H | -1.27812900 | -2.66123800 | -0.35898000 |
| H | -1.96933000 | -1.94305200 | 1.12638200 |
| F | -0.39921600 | -3.76166900 | 1.87914600 |
| F | 1.14456200 | -2.90999100 | 0.61404000 |
| F | 0.42736500 | -1.80458500 | 2.34791300 |

**TS8**

| | | | |
|---|---|---|---|
| C | -2.25552400 | -2.69381900 | 0.12440500 |
| C | -1.57443600 | -1.95184000 | -0.86684500 |
| C | -2.04679500 | -1.86875700 | -2.17576300 |
| C | -3.23130700 | -2.54020200 | -2.48317600 |
| C | -3.92431900 | -3.27375700 | -1.50509700 |
| C | -3.44445800 | -3.36000900 | -0.19973400 |
| C | -1.45804200 | -2.59193300 | 1.32382400 |
| C | -0.36935400 | -1.82417200 | 1.04446100 |

| | | | |
|---|---|---|---|
| H | -1.51553500 | -1.29737800 | -2.93126300 |
| H | -3.62282500 | -2.49358900 | -3.49555200 |
| H | -4.84507200 | -3.78430500 | -1.77418600 |
| H | -3.97909500 | -3.93710100 | 0.55029200 |
| H | -1.66694100 | -3.06426400 | 2.27596600 |
| N | -0.39644200 | -1.38180800 | -0.31121000 |
| C | -0.99576500 | 3.57225000 | -0.59535800 |
| C | -2.07529300 | 3.34691700 | 0.26878300 |
| H | -2.64842600 | 4.21625200 | 0.56750200 |
| C | -2.49492900 | 2.10483100 | 0.78545900 |
| O | -1.96467100 | 0.96906000 | 0.55658900 |
| C | -3.69190500 | 2.05579700 | 1.71277100 |
| H | -4.13930400 | 3.03998400 | 1.87033000 |
| H | -4.44462300 | 1.37709800 | 1.29714500 |
| H | -3.38020100 | 1.64179100 | 2.67818200 |
| C | -0.70384100 | 4.98489400 | -1.05898900 |
| H | -0.73763900 | 5.02416400 | -2.15355800 |
| H | -1.41215400 | 5.71042900 | -0.65272300 |
| H | 0.31089700 | 5.26606700 | -0.75533400 |
| Pd | -0.30685900 | 0.72102000 | -0.63120200 |
| O | -0.18347000 | 2.69807700 | -1.06811300 |
| C | 0.78378900 | -1.51788400 | 1.95590400 |
| C | 0.60842700 | -0.32109400 | 2.88157800 |
| H | 1.71174000 | -1.36140800 | 1.39762800 |
| H | 0.94831200 | -2.37436400 | 2.61836000 |
| F | -0.55728300 | -0.36601300 | 3.55701200 |
| F | 1.60608300 | -0.29703700 | 3.79560800 |
| F | 0.65110900 | 0.86370600 | 2.22739300 |
| C | 3.42381700 | 0.35350000 | -1.10303500 |
| C | 2.92998600 | -1.00605700 | -1.10529200 |
| C | 3.70448900 | -2.04397000 | -0.52473500 |
| C | 4.93722200 | -1.71801200 | -0.00083100 |
| C | 5.43930200 | -0.38095400 | -0.01580600 |
| C | 4.69961300 | 0.64743600 | -0.55249900 |
| C | 2.41178900 | 1.12684900 | -1.68610100 |
| C | 1.34348500 | 0.24226000 | -2.00813400 |
| H | 3.33916600 | -3.06713900 | -0.52372600 |
| H | 5.55577500 | -2.50024500 | 0.43194400 |
| H | 6.42071400 | -0.18404100 | 0.40600700 |
| H | 5.08008100 | 1.66559500 | -0.56036100 |
| H | 2.41638200 | 2.19219500 | -1.87595200 |
| H | 0.69458400 | 0.38756400 | -2.87375700 |
| H | 0.65174100 | -1.52675600 | -0.98524500 |

| | | | |
|---|---|---|---|
| N | 1.70617900 | -1.08878100 | -1.67437100 |

**TS9**

| | | | |
|---|---|---|---|
| C | -1.36996400 | -2.43396000 | 0.17084600 |
| C | -0.25353500 | -3.03550000 | -0.45424100 |
| C | -0.40191400 | -3.98188400 | -1.46756200 |
| C | -1.70096600 | -4.35286500 | -1.81948300 |
| C | -2.81845900 | -3.78909000 | -1.17917200 |
| C | -2.66640400 | -2.82370900 | -0.18383400 |
| C | -0.82416100 | -1.44354100 | 1.09979900 |
| C | 0.58352200 | -1.62511400 | 1.04603300 |
| H | 0.46372100 | -4.42697800 | -1.94930400 |
| H | -1.85100200 | -5.09855800 | -2.59542400 |
| H | -3.81574500 | -4.11010100 | -1.46735600 |
| H | -3.53195700 | -2.37816900 | 0.29864500 |
| H | -1.35327200 | -1.04896900 | 1.95679500 |
| N | 0.93694100 | -2.51905200 | 0.08820400 |
| C | -2.38878800 | 2.65456000 | -1.34278800 |
| C | -3.31376100 | 2.61888400 | -0.28882200 |
| H | -4.11406500 | 3.34824900 | -0.31670400 |
| C | -3.30965500 | 1.72211500 | 0.79345100 |
| O | -2.47506000 | 0.78004500 | 1.00541400 |
| C | -4.39334300 | 1.83851500 | 1.84771800 |
| H | -5.09434100 | 2.64935000 | 1.63670800 |
| H | -4.94432000 | 0.89358700 | 1.91149200 |
| H | -3.92929800 | 2.00935900 | 2.82551000 |
| C | -2.57542900 | 3.67259500 | -2.45062900 |
| H | -2.68318800 | 3.15150000 | -3.40856500 |
| H | -3.44973600 | 4.30698000 | -2.28799300 |
| H | -1.68237500 | 4.30327400 | -2.52351300 |
| Pd | -0.83823800 | 0.37375300 | -0.21353000 |
| O | -1.36335400 | 1.90462300 | -1.49411700 |
| C | 1.66990000 | -1.01743300 | 1.88704900 |
| C | 1.26628500 | 0.08248900 | 2.84849800 |
| H | 2.47180600 | -0.62548800 | 1.25094600 |
| H | 2.11957700 | -1.81205300 | 2.49548900 |
| F | 0.27478100 | -0.30333700 | 3.68403000 |
| F | 2.32433600 | 0.42820200 | 3.61293300 |
| F | 0.84608300 | 1.20429600 | 2.22126900 |
| C | 2.79776300 | 1.30150300 | -1.30633900 |
| C | 3.06873200 | -0.11429700 | -1.21133800 |
| C | 4.36824400 | -0.56723900 | -0.86734500 |
| C | 5.34826800 | 0.37898000 | -0.64870900 |
| C | 5.08937600 | 1.77900100 | -0.75117700 |

| | | | |
|---|---|---|---|
| C | 3.83374300 | 2.24348600 | -1.07128500 |
| C | 1.44265700 | 1.40252500 | -1.64300700 |
| C | 0.92473500 | 0.06859200 | -1.70396400 |
| H | 4.58224700 | -1.63028300 | -0.79894400 |
| H | 6.35411900 | 0.05356000 | -0.39491300 |
| H | 5.90129500 | 2.47832700 | -0.57332300 |
| H | 3.63542100 | 3.30939300 | -1.15144400 |
| H | 0.87915500 | 2.29776800 | -1.85820700 |
| H | 0.12703900 | -0.23685800 | -2.38200900 |
| H | 1.63026300 | -1.97461800 | -0.71497200 |
| N | 1.96063500 | -0.84715000 | -1.47494500 |

**Norborn.**

| | | | |
|---|---|---|---|
| C | -1.19086200 | -0.78133300 | -0.51656100 |
| C | 0.08826400 | -1.12847000 | 0.32322100 |
| C | 0.08733700 | 1.12862200 | 0.32288800 |
| C | -1.19151000 | 0.78044300 | -0.51648600 |
| H | -1.14549300 | -1.20728500 | -1.52326900 |
| H | -2.08827200 | -1.17865300 | -0.02837200 |
| H | -1.14688000 | 1.20643900 | -1.52322000 |
| H | -2.08925700 | 1.17693100 | -0.02818700 |
| C | 0.04090600 | 0.00017800 | 1.38075100 |
| H | 0.91202200 | 0.00069300 | 2.04344900 |
| H | -0.87869500 | -0.00004500 | 1.97961900 |
| C | 1.27947800 | -0.67004800 | -0.50750200 |
| H | 1.92145000 | -1.32836400 | -1.08505400 |
| C | 1.27893000 | 0.67072600 | -0.50776600 |
| H | 1.92047700 | 1.32934800 | -1.08542500 |
| H | 0.12043500 | -2.15753300 | 0.68983400 |
| H | 0.11895200 | 2.15776300 | 0.68935600 |

**$HCO_3^-$**

| | | | |
|---|---|---|---|
| C | -0.15850200 | 0.07287100 | -0.00002400 |
| O | 0.14149200 | 1.29172500 | 0.00002000 |
| O | -1.24203100 | -0.53011400 | -0.00019300 |
| O | 1.00482900 | -0.79896200 | 0.00015900 |
| H | 1.71669600 | -0.13842000 | 0.00025600 |

**$H_2O$**

| | | | |
|---|---|---|---|
| O | 0.00000000 | 0.00000000 | 0.11942600 |
| H | 0.00000000 | 0.76261700 | -0.47770500 |
| H | 0.00000000 | -0.76261700 | -0.47770500 |

**$CO_2$**

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| O | 0.00000000 | 0.00000000 | 1.16958400 |
| O | 0.00000000 | 0.00000000 | -1.16958400 |

**acac$^-$**

| | | | |
|---|---|---|---|
| C | -1.27643300 | 0.08950800 | 0.00015400 |
| C | -0.00001000 | -0.54185800 | 0.00048400 |
| H | 0.00001200 | -1.63052800 | 0.00050900 |
| C | 1.27642600 | 0.08950900 | 0.00003600 |
| O | 1.54887900 | 1.30471000 | -0.00029900 |
| C | 2.49505600 | -0.87591300 | -0.00004200 |
| H | 2.23150400 | -1.94131900 | 0.00014500 |
| H | 3.11843800 | -0.66863600 | -0.88068600 |
| H | 3.11877200 | -0.66842300 | 0.88031900 |
| C | -2.49504400 | -0.87590300 | -0.00032500 |
| H | -3.11840000 | -0.66822900 | -0.88088600 |
| H | -2.23150500 | -1.94131900 | -0.00062600 |
| H | -3.11878200 | -0.66884000 | 0.88011900 |
| O | -1.54888000 | 1.30469500 | 0.00020700 |

**$CF_3CH_2I$**

| | | | |
|---|---|---|---|
| C | -1.74696900 | -0.00671500 | 0.00000000 |
| C | -0.57949900 | 0.95977000 | 0.00000700 |
| H | -0.61679000 | 1.57789800 | -0.89488800 |
| H | -0.61678600 | 1.57789000 | 0.89490800 |
| F | -1.76238800 | -0.79452000 | -1.08799900 |
| F | -1.76239000 | -0.79454100 | 1.08798600 |
| F | -2.89174400 | 0.71491300 | 0.00000700 |
| I | 1.37624700 | -0.01899600 | 0.00000000 |

**$I^-$**

| | | | |
|---|---|---|---|
| I | 0.00000000 | 0.00000000 | 0.00000000 |