

Supporting Information

A Diversity-Oriented Synthesis of Bioactive Benzanilides by a Regioselective C(sp²)-H Hydroxylation Strategy

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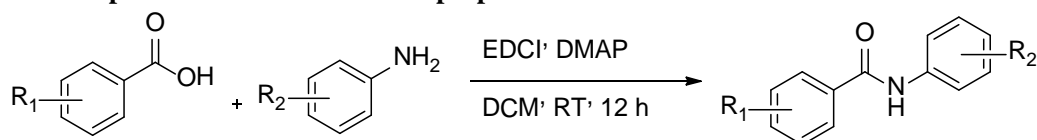
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Experimental part:

Materials and Methods

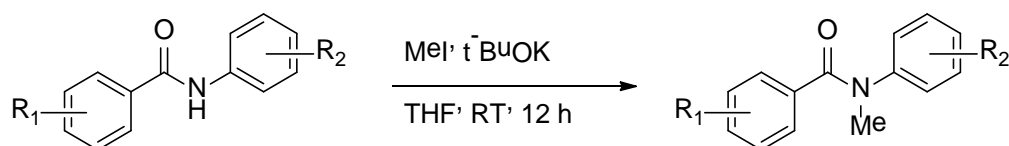
All commercial materials (Alfa Aesar, Aladdin, J&K Chemical LTD, Energy Chemical.) were used without further purification. All solvents were analytical grade. The potassium persulfate and potassium carbonate were ground to powder. All benzoic acids, anilines, *N*-methylanilines, benzyl bromide were purchased. The 2-deuteriobenzoic acid was prepared by Daugulis' procedure^[1]. The 2-deuterioaniline was prepared by Xi's procedure^[2]. The ¹H NMR and ¹³C NMR spectra were recorded on a Bruker AVANCE^{III} 400 MHz spectrometer in CD₃OD, CDCl₃ or (CD₃)₂SO using solvent peak as a standard. All ¹³C NMR spectra were recorded with complete proton decoupling. Low-resolution mass spectral analyses were performed with an Agilent 6340 or Waters AQUITY UPLCTM/MS. All reactions were carried out in sealed tube with Teflon cap. Analytical TLC was performed on Yantai Chemical Industry Research Institute silica gel 60 F254 plates and flash column chromatography was performed on Qingdao Haiyang Chemical Co. Ltd silica gel 60 (200-300mesh). The rotavapor was BUCHI's Rotavapor R-3.

General procedure for benzanilides preparation^[3]



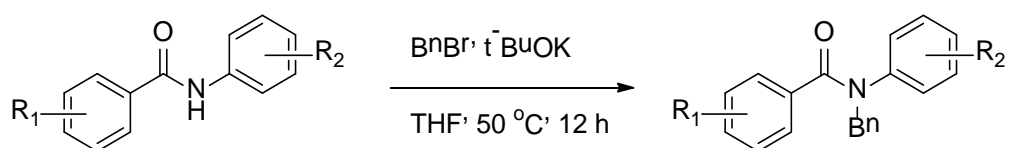
A mixture of benzoic acid (15 mmol), EDCI (16.5 mmol), DMAP (1.5 mmol) in DCM (30 ml) was stirred in a round bottom flask at room temperature for 15 min. Then, aniline (13.5 mmol) was added slowly. The reaction mixture was stirred for 12 h at room temperature. The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO₃, extracted with DCM. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by filtration.

General procedure for *N*-methyl-benzanilides preparation^[4]



A mixture of benzanilide (8 mmol) and t-BuOK (9.6 mmol) in THF (20 ml) was stirred in a round bottom flask at room temperature for 15 min. Then, MeI (9.6 mmol) was added slowly. The reaction mixture was stirred for 12 h at room temperature. The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO₃, extracted by DCM. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate = 4: 1) to give the *N*-methyl-benzanilide.

General procedure for *N*-benzyl-benzanilides preparation^[4]



A mixture of benzanilide (2 mmol) and t-BuOK (2.4 mmol) in THF (10 ml) was stirred in a round bottom flask at room temperature for 15 min. Then, BnBr (2.4 mmol) was added slowly. The reaction mixture was stirred for 12 h

at 50 °C. The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO₃, extracted by DCM. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate = 6: 1) to give the *N*-benzyl-benzanilide.

I General procedure for ruthenium-catalyzed hydroxylation of benzanilides

To a 15 ml sealed-tube were added benzanilide (0.10 mmol, 1.0 equiv), K₂S₂O₈ (0.30 mmol, 3.0 equiv), [Ru(*p*-cymene)Cl₂]₂ (0.005 mmol, 0.05 equiv) and TFAA (0.1 ml). The mixture was stirred at room temperature for 2 min. Then, TFA (0.9 ml) was added. The tube was sealed and heated. The reaction was monitored by TLC (n-hexane: acetone = 4: 1). After completion of the reaction, dichloromethane was added to dilute the reaction mixture and saturated aqueous NaHCO₃ was added to neutralize TFA and TFAA. Then the organic layer was dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. Finally, the residue was purified by silica gel column chromatography to give the desired product.

II General procedure for palladium-catalyzed hydroxylation of benzanilides

To a 15 ml sealed-tube were added benzanilide (0.10 mmol, 1.0 equiv), K₂S₂O₈ (0.20 mmol, 2.0 equiv), Pd(OAc)₂ (0.01 mmol, 0.1 equiv) and TFAA (0.1 ml). The mixture was stirred at room temperature for 2 min. Then, TFA (0.9 ml) was added. The tube was sealed and heated. The reaction was monitored by TLC (n-hexane: acetone = 4: 1). After completion of the reaction, dichloromethane was added to dilute the reaction mixture and saturated aqueous NaHCO₃ was added to neutralize TFA and TFAA. Then the organic layer was dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. Finally, the residue was purified by silica gel column chromatography to give the desired product.

Procedure for gram scale reactions

1. 2-Hydroxy-*N*-methyl-*N*-phenylbenzamide (**2b**)

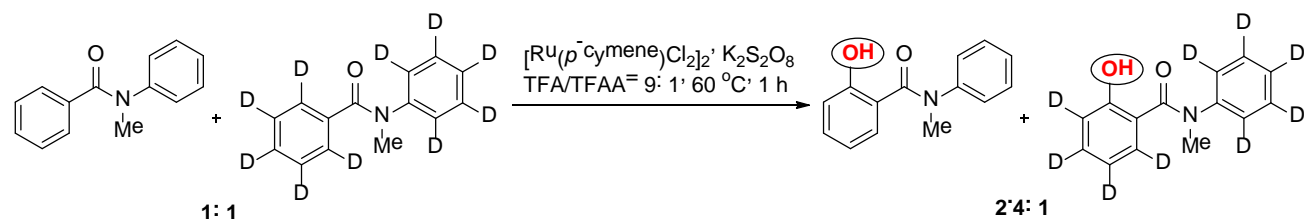
To a 100 mL round bottom flask, following the general procedure **I**, *N*-methyl-benzanilide (2.0 g, 9.48 mmol), K₂S₂O₈ (7.7 g, 28.44 mmol), [Ru(*p*-cymene)Cl₂]₂ (145 mg, 0.24 mmol), TFAA (8 ml) and TFA (70 ml) were used. The reaction mixture was stirred at 60 °C for 12 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate = 10: 1). Finally, compound (**2b**) (1.9 g) was isolated in 90% yield.

2. *N*-(2-hydroxyphenyl)-*N*-methylbenzamide (**2a**)

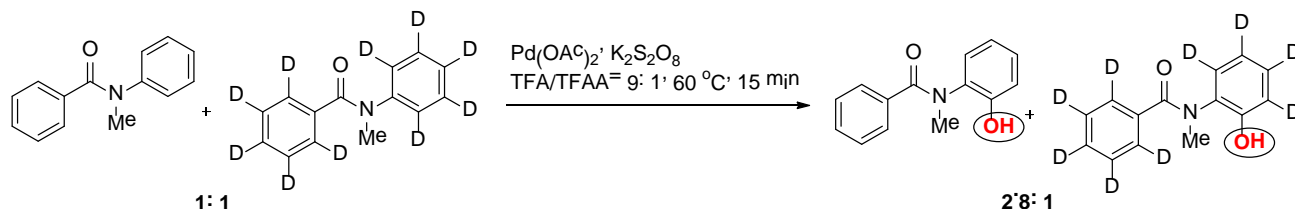
To a 100 mL round bottom flask, following the general procedure **II**, *N*-methyl-benzanilide (2.0 g, 9.48 mmol), K₂S₂O₈ (7.7 g, 28.44 mmol) or Pd(OAc)₂ (107 mg, 0.47 mmol), TFAA (8 ml) and TFA (70 ml) were used. The reaction mixture was stirred at 60 °C for 1.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate = 4: 1). Finally, compound (**2a**) (1.3 g) was isolated in 61% yield.

Procedure for preliminary mechanistic study

1. Intermolecular Experiments

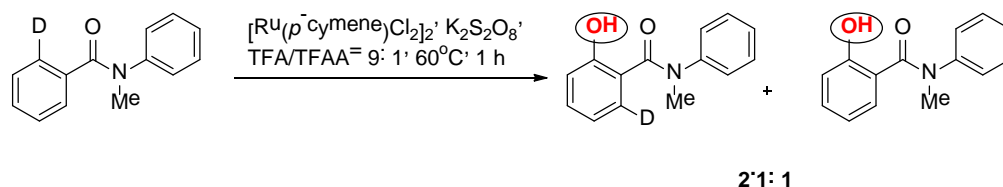


To a 15 ml sealed-tube were added *N*-methyl-benzanilide (10.6 mg, 0.05 mmol), *N*-methyl-benzanilide – d10 (11.1 mg, 0.05 mmol), $K_2S_2O_8$ (54 mg, 0.20 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (3.1 mg, 0.005 mmol), TFAA (0.1 ml). The mixture was stirred at room temperature for 2 min. Then, TFA (0.9 ml) was added. The tube was sealed and heated at 60 °C for 1 h. The reaction mixture was cooled to room temperature. Then dichloromethane was added to dilute the reaction mixture and saturated aqueous $NaHCO_3$ was added to neutralize TFA and TFAA. The organic layer was dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1) 1H -NMR shows $k_H/k_D = 2.4: 1$.

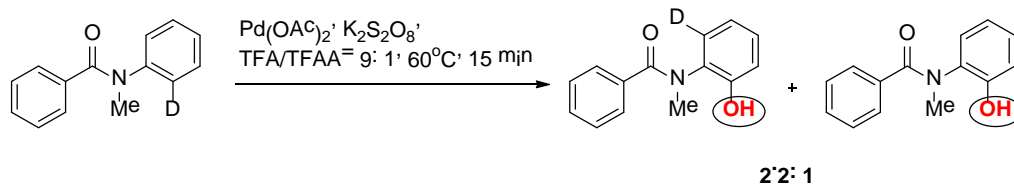


To a 15 ml sealed-tube were added *N*-methyl-benzanilide (10.6 mg, 0.05 mmol), *N*-methyl-benzanilide – d10 (11.1 mg, 0.05 mmol), $K_2S_2O_8$ (54 mg, 0.20 mmol), $Pd(OAc)_2$ (2.3 mg, 0.01 mmol), TFAA (0.1 ml). The mixture was stirred at room temperature for 2 min. Then, TFA (0.9 ml) was added. The tube was sealed and heated at 60 °C for 15 min. The reaction mixture was cooled to room temperature. Then dichloromethane was added to dilute the reaction mixture and saturated aqueous $NaHCO_3$ was added to neutralize TFA and TFAA. The organic layer was dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silica gel column chromatography (n-hexane: acetone= 6: 1) 1H -NMR shows $k_H/k_D = 2.8: 1$.

2. Intramolecular Experiments



To a 15 ml sealed-tube were added 2-deuterio-*N*-methyl-*N*-phenylbenzamide (21 mg, 0.10 mmol), $K_2S_2O_8$ (54 mg, 0.20 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (3.1 mg, 0.005 mmol), TFAA (0.1 ml). The mixture was stirred at room temperature for 2 min. Then, TFA (0.9 ml) was added. The tube was sealed and heated at 60 °C for 1 h. The reaction mixture was cooled to room temperature. Then dichloromethane was added to dilute the reaction mixture and saturated aqueous $NaHCO_3$ was added to neutralize TFA and TFAA. The organic layer was dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1) 1H -NMR shows $k_H/k_D = 2.1: 1$.



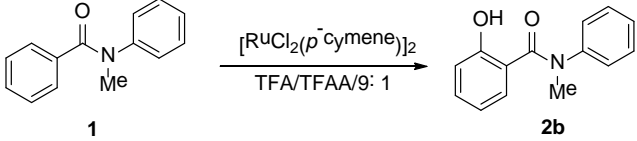
To a 15 ml sealed-tube were added *N*-(2-deuteriophenyl)-*N*-methylbenzamide (21 mg, 0.10 mmol), $K_2S_2O_8$ (54 mg, 0.20 mmol), $Pd(OAc)_2$ (2.3 mg, 0.01 mmol), TFAA (0.1 ml). The mixture was stirred at room temperature for 2 min. Then, TFA (0.9 ml) was added. The tube was sealed and heated at 60 °C for 15 min. The reaction mixture was cooled to room temperature. Then dichloromethane was added to dilute the reaction mixture and saturated aqueous $NaHCO_3$ was added to neutralize TFA and TFAA. The organic layer was dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silica gel column chromatography

(n-hexane: acetone= 6: 1) ¹H-NMR shows k_H/k_D = 2.2: 1.

References

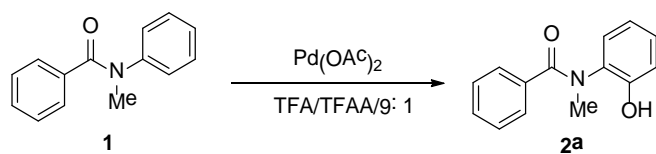
- (1) H. A. Chiong, Q. N. Pham and O. Daugilis, *J. Am. Chem. Soc.*, 2007, **129**, 9879.
- (2) Y. Chi, W. X. Zhang and Z. F. Xi, *Org. Lett.*, 2014, **16**, 6274.
- (3) X. Q. Hao, L. J. Chen, B. Z. Ren, L. Y. Li, X. Y. Yang, J. F. Gong, J. L. Niu and M. P. Song, *Org. Lett.*, 2014, **16**, 1104.
- (4) T. Y. Luh and S. H. Fung, *Synthetic Communications*, 1979, **9**, 757.

Table S1. Optimization of the Reaction Conditions with [Ru(*p*-cymene)Cl₂]₂ as Catalyst



entry	equiv of catalyst	oxidant	condition	yield ^a (%)
1	0.05	K ₂ S ₂ O ₈ (3.0 eq)	60 °C: 5 h	87
2	0.05	K ₂ S ₂ O ₈ (3.0 eq)	60 °C: 7 h	85
3	0.025	K ₂ S ₂ O ₈ (3.0 eq)	60 °C: 6 h	67
4	0.01	K ₂ S ₂ O ₈ (3.0 eq)	60 °C: 6 h	57
5	0.05	K ₂ S ₂ O ₈ (2.0 eq)	60 °C: 6 h	70
6	0.05	K ₂ S ₂ O ₈ (1.5 eq)	60 °C: 6 h	28
7	0.05	K ₂ S ₂ O ₈ (3.0 eq)	25 °C: 6 h	0
8	0.05	K ₂ S ₂ O ₈ (3.0 eq)	50 °C: 6 h	49
9	0.05	K ₂ S ₂ O ₈ (3.0 eq)	70 °C: 6 h	65
10	0.05	K ₂ S ₂ O ₈ (3.0 eq)	80 °C: 6 h	28
11	0.05	selectfluor(3.0 eq)	60 °C: 6 h	0
12	0.05	NFPy-TfO(3.0 eq)	60 °C: 6 h	0
13	0.05	NaIO ₄ (3.0 eq)	60 °C: 6 h	0
14	0.05	PhI(OAc) ₂ (3.0 eq)	60 °C: 6 h	trace
15	0.05	Na ₂ S ₂ O ₈ (3.0 eq)	60 °C: 6 h	0
16	0.05	(NH ₄) ₂ S ₂ O ₈ (3.0 eq)	60 °C: 6 h	58
17	0.05	KIO ₃ (3.0 eq)	60 °C: 6 h	trace

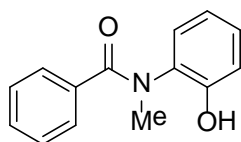
^a Conversion ratio.

Table S2. Optimization of the Reaction Conditions with Pd(OAc)₂ as Catalyst

entry	equiv of catalyst	oxidant	condition	yield ^a (%)
1	0.1	K ₂ S ₂ O ₈ (2.0 eq)	60 °C: 20 min	52
2	0.1	K ₂ S ₂ O ₈ (2.0 eq)	60 °C: 1 h	61
3	0.05	K ₂ S ₂ O ₈ (2.0 eq)	60 °C: 0.5 h	42
4	0.025	K ₂ S ₂ O ₈ (2.0 eq)	60 °C: 0.5 h	18
5	0.1	K ₂ S ₂ O ₈ (1.5 eq)	60 °C: 0.5 h	31
6	0.1	K ₂ S ₂ O ₈ (1.0 eq)	60 °C: 0.5 h	15
7	0.1	K ₂ S ₂ O ₈ (2.0 eq)	25 °C: 0.5 h	28
8	0.1	K ₂ S ₂ O ₈ (2.0 eq)	50 °C: 0.5 h	50
9	0.1	K ₂ S ₂ O ₈ (2.0 eq)	70 °C: 0.5 h	16
10	0.1	K ₂ S ₂ O ₈ (2.0 eq)	80 °C: 0.5 h	9
11	0.1	selecfuor(2.0 eq)	60 °C: 0.5 h	trace
12	0.1	NFPy TfO(2.0 eq)	60 °C: 0.5 h	30
13	0.1	NaIO ₄ (2.0 eq)	60 °C: 0.5 h	27
14	0.1	PhI(OAc) ₂ (2.0 eq)	60 °C: 0.5 h	16
15	0.1	Na ₂ S ₂ O ₈ (2.0 eq)	60 °C: 0.5 h	0
16	0.1	(NH ₄) ₂ S ₂ O ₈ (2.0 eq)	60 °C: 0.5 h	0
17	0.1	KIO ₃ (2.0 eq)	60 °C: 0.5 h	0

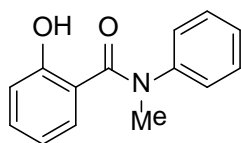
^a Conversion ratio.

Data of products



N-(2-hydroxyphenyl)-*N*-methylbenzamide (**2a**)

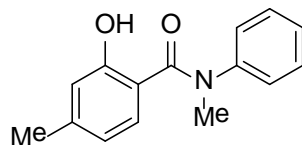
Following the general procedure **II**, *N*-methyl-*N*-phenylbenzamide (22 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 0.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**2a**) (16 mg) was isolated in 70% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.32 (d, *J* = 7.52 Hz, 2H), 7.22 (t, *J* = 7.00 Hz, 1H), 7.15 (t, *J* = 7.40 Hz, 2H), 7.02 (t, *J* = 7.64 Hz, 1H), 6.93 (d, *J* = 7.76 Hz, 1H), 6.76 (d, *J* = 8.08 Hz, 1H), 6.65 (t, *J* = 7.52 Hz, 1H), 3.34 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 174.1, 154.0, 137.6, 132.9, 130.7, 130.4, 130.1, 128.8, 128.6, 120.8, 117.4, 37.2; LRMS (ESI) calcd for C₁₄H₁₃NO₂[M+H]⁺: 228.09, found 228.38.



2-Hydroxy-*N*-methyl-*N*-phenylbenzamide (**2b**)

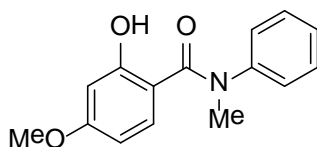
Following the general procedure **I**, *N*-methyl-*N*-phenylbenzamide (22 mg, 0.1mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The

reaction mixture was stirred at 60 °C in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**2b**) (21 mg) was isolated in 93% yield. ¹H-NMR (400 MHz, (CD₃)₂CO) δ (ppm) 10.51 (s, 1H), 7.35 (t, *J* = 7.52 Hz, 2H), 7.24 - 7.27 (m, 3H), 7.16 (t, *J* = 7.68 Hz, 1H), 6.80 – 6.84 (m, 2H), 6.46 (t, *J* = 7.48 Hz, 1H), 3.44 (s, 3H); ¹³C-NMR (100 MHz, (CD₃)₂CO) δ (ppm) 171.6, 160.2, 146.1, 132.9, 130.9, 130.3, 127.9, 127.8, 119.1, 118.7, 118.7, 118.0, 117.9, 39.1; LRMS (ESI) calcd for C₁₄H₁₃NO₂[M+H]⁺: 228.09, found 228.38.



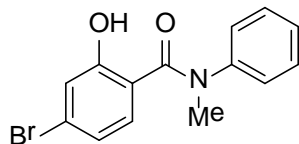
2-Hydroxy-N,4-dimethyl-N-phenylbenzamide (**3a**)

Following the general procedure **I**, *N*,4-dimethyl-*N*-phenylbenzamide (23 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3a**) (22 mg) was isolated in 91% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.25 (t, *J* = 7.64 Hz, 2H), 7.16 – 7.20 (m, 3H), 6.85 (d, *J* = 7.80 Hz, 1H), 6.52 (s, 1H), 6.44 (d, *J* = 7.84 Hz, 1H), 3.41 (s, 3H), 2.17 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.7, 156.5, 145.6, 142.8, 130.0, 129.9, 128.1, 127.9, 120.9, 120.6, 117.4, 38.5, 21.4; LRMS (ESI) calcd for C₁₅H₁₅NO₂[M+H]⁺: 242.11, found 242.42.



2-Hydroxy-4-methoxy-N-methyl-N-phenylbenzamide (**3b**)

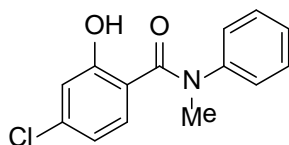
Following the general procedure **I**, 4-methoxy-*N*-methyl-*N*-phenylbenzamide (25 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3b**) (22 mg) was isolated in 86% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.29 (t, *J* = 7.56 Hz, 2H), 7.17 – 7.22 (m, 3H), 6.84 (d, *J* = 8.68 Hz, 1H), 6.27 (d, *J* = 2.32 Hz, 1H), 6.14 (dd, *J* = 8.72 Hz, *J* = 2.32 Hz, 1H), 3.68 (s, 3H), 3.41 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.7, 163.8, 159.7, 146.1, 131.7, 130.2, 128.0, 127.9, 114.8, 106.0, 102.1, 49.0, 38.8; LRMS (ESI) calcd for C₁₅H₁₅NO₃[M+H]⁺: 258.11, found 258.41.



4-Bromo-2-hydroxy-N-methyl-N-phenylbenzamide (**3c**)

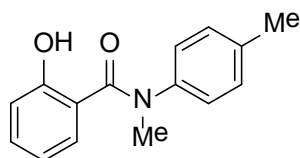
Following the general procedure **I**, 4-bromo-*N*-methyl-*N*-phenylbenzamide (29 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 4 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3c**) (22 mg) was isolated in 72% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.26 (t, *J* = 8.08 Hz, 2H), 7.17 - 7.21 (m, 3H), 6.94 (d, *J* = 8.04 Hz, 1H), 6.84 (s, 1H), 6.80 (d, *J* = 8.00 Hz, 1H), 3.41 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 171.3, 156.6, 145.0, 131.1, 130.0, 128.4, 127.9, 124.7, 124.1, 122.9, 120.0, 38.2; LRMS (ESI) calcd for

$C_{14}H_{12}BrNO_2[M+H]^+$: 306.01, found 306.29.



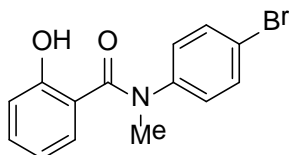
4-Chloro-2-hydroxy-*N*-methyl-*N*-phenylbenzamide (**3d**)

Following the general procedure **I**, 4-chloro-*N*-methyl-*N*-phenylbenzamide (25 mg, 0.1 mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 7 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3d**) (19 mg) was isolated in 73% yield. 1H -NMR (400 MHz, CD_3OD) δ (ppm) 7.26 (t, J = 8.16 Hz, 2H), 7.17 – 7.21 (m, 3H), 7.00 (d, J = 8.08 Hz, 1H), 6.68 (s, 1H), 6.65 (d, J = 8.48 Hz, 1H), 3.42 (s, 3H); ^{13}C -NMR (100 MHz, CD_3OD) δ (ppm) 171.3, 156.7, 145.0, 136.9, 130.9, 130.1, 128.3, 127.9, 123.7, 119.9, 116.8, 38.2; LRMS (ESI) calcd for $C_{14}H_{12}ClNO_2[M+H]^+$: 262.06, found 262.31.



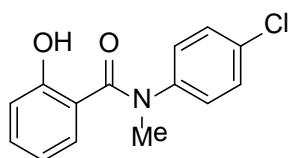
2-Hydroxy-*N*-methyl-*N*-(*p*-tolyl)benzamide (**3e**)

Following the general procedure **I**, *N*-methyl-*N*-(*p*-tolyl)benzamide (23 mg, 0.1 mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3e**) (19 mg) was isolated in 81% yield. 1H -NMR (400 MHz, CD_3OD) δ (ppm) 7.09 – 6.98 (m, 6H), 6.68 (d, J = 8.20 Hz, 1H), 6.63 (t, J = 7.32 Hz, 1H), 3.39 (s, 3H), 2.24 (s, 3H); ^{13}C -NMR (100 MHz, CD_3OD) δ (ppm) 172.4, 155.9, 142.7, 138.2, 131.8, 130.5, 129.7, 127.6, 124.5, 119.8, 116.8, 38.4, 21.0; LRMS (ESI) calcd for $C_{15}H_{15}NO_2[M+H]^+$: 242.11, found 242.37.



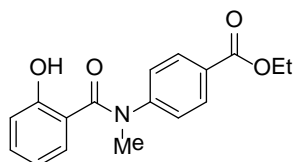
N-(4-bromophenyl)-2-hydroxy-*N*-methylbenzamide (**3f**)

Following the general procedure **I**, *N*-(4-bromophenyl)-*N*-methylbenzamide (29 mg, 0.1 mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3f**) (23 mg) was isolated in 75% yield. 1H -NMR (400 MHz, CD_3OD) δ (ppm) 7.38 (d, J = 8.64 Hz, 2H), 7.13 (d, J = 8.64 Hz, 2H), 7.06 - 7.14 (m, 2H), 6.67 – 6.73 (m, 2H), 3.40 (s, 3H); ^{13}C -NMR (100 MHz, CD_3OD) δ (ppm) 172.2, 155.5, 144.5, 133.0, 132.0, 129.8, 129.7, 124.6, 121.4, 120.1, 116.8, 38.1; LRMS (ESI) calcd for $C_{14}H_{12}BrNO_2[M+H]^+$: 306.01, found 306.29.



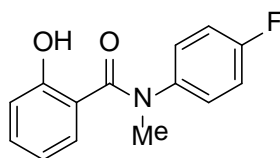
***N*-(4-chlorophenyl)-2-hydroxy-*N*-methylbenzamide (3g)**

Following the general procedure I, *N*-(4-chlorophenyl)-*N*-methylbenzamide (25 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (3g) (24.5 mg) was isolated in 94% yield. ¹H-NMR (400 MHz, (CD₃)₂SO) δ (ppm) 7.28 (d, *J* = 8.00 Hz, 2H), 7.21 (d, *J* = 8.00 Hz, 2H), 7.05 – 7.09 (m, 2H), 6.66 – 6.70 (m, 2H), 3.29 (s, 3H); ¹³C-NMR (100 MHz, (CD₃)₂SO) δ (ppm) 168.3, 153.3, 142.7, 130.5, 130.1, 128.4, 128.3, 128.2, 124.4, 118.5, 115.6, 36.8; LRMS (ESI) calcd for C₁₄H₁₂ClNO₂[M+H]⁺: 262.06, found 262.36.



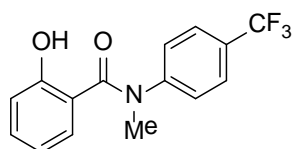
Ethyl 4-(2-hydroxy-*N*-methylbenzamido)benzoate (3h)

Following the general procedure I, ethyl 4-(*N*-methylbenzamido)benzoate (29 mg, 0.1mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 4 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (3h) (27.4 mg) was isolated in 92% yield. ¹H-NMR (400 MHz, (CD₃)₂SO) δ (ppm) 9.70 (s, 1H), 7.79 (d, *J* = 8.00 Hz, 2H), 7.32 (d, *J* = 8.00 Hz, 2H), 7.08 – 7.11 (m, 2H), 6.66 – 6.71 (m, 2H), 4.26 (q, *J* = 8.00 Hz, 2H), 3.34 (s, 3H), 1.28 (t, *J* = 8.00 Hz, 3H); ¹³C-NMR (100 MHz, (CD₃)₂SO) δ (ppm) 168.4, 165.1, 153.4, 148.0, 130.4, 129.4, 128.5, 127.1, 126.1, 124.3, 118.6, 115.6, 60.7, 36.7, 14.1; LRMS (ESI) calcd for C₁₇H₁₇NO₄[M+H]⁺: 300.12, found 300.43.



***N*-(4-fluorophenyl)-2-hydroxy-*N*-methylbenzamide (3i)**

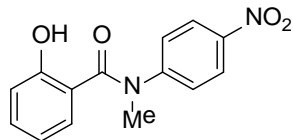
Following the general procedure I, *N*-(4-fluorophenyl)-*N*-methylbenzamide (23 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (3i) (20 mg) was isolated in 82% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.23 (dd, *J* = 8.60 Hz, *J* = 4.88 Hz, 2H), 7.10 (t, *J* = 7.52 Hz, 1H), 7.05 (d, *J* = 7.28 Hz, 1H), 6.94 – 6.98 (m, 2H), 6.66 – 6.71 (m, 2H), 3.40 (s, 3H); ¹³C-NMR (100 MHz, (CD₃)₂CO) δ (ppm) 171.6, 162.6 (d, *J*_{C-F} = 244 Hz), 155.4, 141.4 131.8, 129.9 (d, *J*_{C-F} = 8 Hz), 129.6, 124.7, 120.0, 116.7 (d, *J*_{C-F} = 14 Hz), 116.4, 38.3; LRMS (ESI) calcd for C₁₄H₁₂FNO₂[M+H]⁺: 246.09, found 246.37.



2-Hydroxy-*N*-methyl-*N*-(4-(trifluoromethyl)phenyl)benzamide (3j)

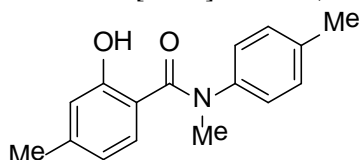
Following the general procedure I, *N*-methyl-*N*-(4-(trifluoromethyl)phenyl)benzamide (28 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (3j) (28

mg) was isolated in 95% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.54 (d, *J* = 8.40 Hz, 2H), 7.39 (d, *J* = 8.36 Hz, 2H), 7.11 – 7.15 (m, 2H), 6.73 (t, *J* = 7.52 Hz, 1H), 6.68 (d, *J* = 8.08 Hz, 1H), 3.45 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.2, 155.4, 148.7, 132.3, 129.8, 129.6 (q, *J*_{C-F} = 32 Hz), 128.4, 126.8 (q, *J*_{C-F} = 4 Hz), 125.4 (q, *J*_{C-F} = 270 Hz), 124.4, 120.2, 116.8, 37.9; LRMS (ESI) calcd for C₁₅H₁₂F₃NO₂[M+H]⁺: 296.08, found 296.39.



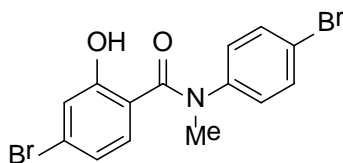
2-Hydroxy-*N*-methyl-*N*-(4-nitrophenyl)benzamide (**3k**)

Following the general procedure **I**, *N*-methyl-*N*-(4-nitrophenyl)benzamide (26 mg, 0.1mmol), K₂S₂O₈ (81 mg, 0.3mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3k**) (19.2 mg) was isolated in 71 % yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.33 (s, 1H), 8.17 (d, *J*= 8.92 Hz, 2H), 7.22 – 7.27 (m, 3H), 6.97 (d, *J* = 8.32 Hz, 1H), 6.68 (dd, *J* = 7.96 Hz, *J* = 1.08 Hz, 1H), 7.40 (t, *J* = 8.32 Hz, 1H), 3.55 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 172.1, 160.6, 160.4, 151.0, 145.7, 133.7, 130.3, 126.8, 125.1, 118.4, 118.4, 115.6, 39.5; LRMS (ESI) calcd for C₁₄H₁₂N₂O₄[M+H]⁺: 273.08, found 273.38.



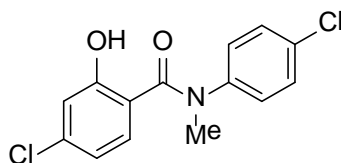
2-Hydroxy-*N*,4-dimethyl-*N*-(*p*-tolyl)benzamide (**3l**)

Following the general procedure **I**, *N*-4-dimethyl-*N*-(*p*-tolyl)benzamide (24 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 4 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3l**) (21 mg) was isolated in 82% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.06 (s, 4H), 6.84 (d, *J* = 7.80 Hz, 1H), 6.52 (s, 1H), 6.43 (d, *J* = 7.76 Hz, 1H), 3.38 (s, 3H), 2.26 (s, 3H), 2.17 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.7, 156.5, 143.0, 142.7, 138.1, 130.6, 129.8, 127.6, 120.9, 120.6, 117.4, 38.6, 21.3, 21.0; LRMS (ESI) calcd for C₁₆H₁₇NO₂[M+H]⁺: 256.13, found 256.41.



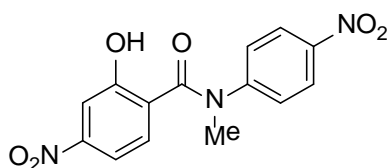
4-Bromo-*N*-(4-bromophenyl)-2-hydroxy-*N*-methylbenzamide (**3m**)

Following the general procedure **I**, 4-bromo-*N*-(4-bromophenyl)-*N*-methylbenzamide (37 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3m**) (28 mg) was isolated in 73% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.40 (d, *J* = 8.52 Hz, 2H), 7.12 (d, *J* = 8.44 Hz, 2H), 7.00 (d, *J* = 7.96 Hz, 1H), 6.86 – 6.88 (m, 2H), 3.39 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 171.1, 156.3, 144.1, 133.1, 131.1, 129.8, 125.0, 124.1, 123.2, 121.7, 119.8, 38.0; LRMS (ESI) calcd for C₁₄H₁₁Br₂NO₂[M+H]⁺: 383.92, found 384.24.



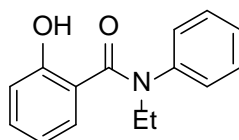
4-Chloro-*N*-(4-chlorophenyl)-2-hydroxy-*N*-methylbenzamide (**3n**)

Following the general procedure **I**, 4-chloro-*N*-(4-chlorophenyl)-*N*-methylbenzamide (28 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TF₃AA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 9 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3n**) (21 mg) was isolated in 71% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 11.05 (s, 1H), 7.32 (d, *J* = 8.00 Hz, 2H), 7.05 (d, *J* = 8.00 Hz, 2H), 6.96 (d, *J* = 4.00 Hz, 1H), 6.58 (d, *J* = 8.00 Hz, 1H), 6.43 (dd, *J* = 8.00 Hz, *J* = 4.00 Hz, 1H), 3.45 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.0, 161.8, 143.6, 138.8, 133.3, 131.3, 130.2, 128.0, 118.6, 118.4, 114.2, 39.5; LRMS (ESI) calcd for C₁₄H₁₁Cl₂NO₂[M+H]⁺: 296.02, found 296.34.



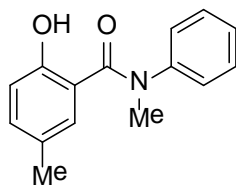
2-Hydroxy-*N*-methyl-4-nitro-*N*-(4-nitrophenyl)benzamide (**3o**)

Following the general procedure **I**, *N*-methyl-4-nitro-*N*-(4-nitrophenyl)benzamide (31 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TF₃AA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 90 °C. in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3o**) (27 mg) was isolated in 85% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.13 (d, *J* = 8.92 Hz, 2H), 7.65 (dd, *J* = 8.36 Hz, *J* = 1.56 Hz, 1H), 7.45 – 7.50 (m, 4H), 3.50 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 169.7, 155.7, 150.8, 150.1, 147.5, 131.3, 130.9, 128.6, 125.2, 115.2, 111.4, 37.6; LRMS (ESI) calcd for C₁₄H₁₁N₃O₆[M+H]⁺: 318.06, found 318.33.



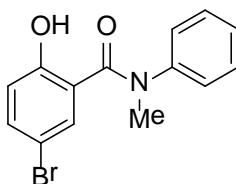
N-ethyl-2-hydroxy-*N*-phenylbenzamide (**3p**)

Following the general procedure **I**, *N*-ethyl-*N*-phenylbenzamide (23 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TF₃AA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3p**) (23 mg) was isolated in 95% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.15 – 7.26 (m, 5H), 7.05 (t, *J* = 7.60 Hz, 1H), 6.98 (d, *J* = 7.32 Hz, 1H), 6.66 (d, *J* = 8.16 Hz, 1H), 6.61 (t, *J* = 7.36 Hz, 1H), 3.91 (q, *J* = 7.08 Hz, 2H), 1.19 (t, *J* = 7.12 Hz, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.0, 155.8, 143.5, 131.7, 129.9, 129.7, 129.0, 128.3, 124.7, 119.7, 116.8, 46.0, 13.2; LRMS (ESI) calcd for C₁₅H₁₅NO₂[M+H]⁺: 242.11, found 242.37.



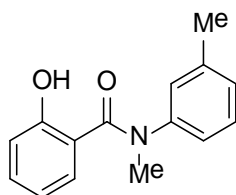
2-Hydroxy-*N*,5-dimethyl-*N*-phenylbenzamide (**3q**)

Following the general procedure **I**, *N*,3-dimethyl-*N*-phenylbenzamide (23 mg, 0.1 mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 5.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3q**) (18 mg) was isolated in 74% yield. 1H -NMR (400 MHz, CD_3OD) δ (ppm) 7.15 - 7.27 (m, 5H), 6.89 (d, J = 8.20 Hz, 1H), 6.82 (s, 1H), 6.57 (d, J = 8.28 Hz, 1H), 3.41 (s, 3H), 2.08 (s, 3H); ^{13}C -NMR (100 MHz, CD_3OD) δ (ppm) 172.5, 153.5, 145.3, 132.4, 129.9, 129.9, 129.1, 128.1, 127.9, 124.1, 116.7, 38.4, 20.2; LRMS (ESI) calcd for $C_{15}H_{15}NO_2[M+H]^+$: 242.11, found 242.37.



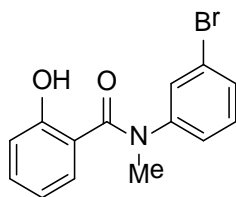
5-Bromo-2-hydroxy-*N*-methyl-*N*-phenylbenzamide (**3r**)

Following the general procedure **I**, 3-bromo-*N*-methyl-*N*-phenylbenzamide (29 mg, 0.1 mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3r**) (21 mg) was isolated in 72% yield. 1H -NMR (400 MHz, $CDCl_3$) δ (ppm) 10.96 (s, 1H), 7.30 - 7.40 (m, 3H), 7.23 (dd, J = 8.80 Hz, J = 2.28 Hz, 1H), 7.12 (d, J = 7.60 Hz, 2H), 6.81 (d, J = 8.84 Hz, 1H), 6.71 (d, J = 1.60 Hz, 1H), 3.49 (s, 3H); ^{13}C -NMR (100 MHz, $CDCl_3$) δ (ppm) 170.1, 159.9, 159.6, 144.6, 135.6, 133.1, 130.1, 127.9, 126.7, 119.8, 119.7, 117.5, 109.4, 39.4; LRMS (ESI) calcd for $C_{14}H_{12}BrNO_2[M+H]^+$: 306.01, found 306.29.



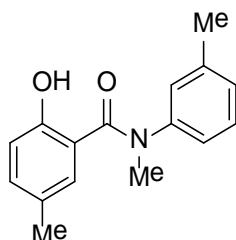
2-Hydroxy-*N*-methyl-*N*-(*m*-tolyl)benzamide (**3s**)

Following the general procedure **I**, *N*-methyl-*N*-(*m*-tolyl)benzamide (23 mg, 0.1 mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 10h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3s**) (13 mg) was isolated in 54% yield. 1H -NMR (400 MHz, CD_3OD) δ (ppm) 6.98 - 7.13(m, 6H), 6.69 (d, J = 8.20 Hz, 1H), 6.64 (t, J = 7.40 Hz, 1H), 3.40 (s, 3H), 2.24 (s, 3H); ^{13}C -NMR (100 MHz, CD_3OD) δ (ppm) 172.4, 156.0, 145.2, 140.2, 131.8, 129.8, 129.7, 128.8, 128.4, 124.8, 124.4, 119.8, 116.8, 38.4, 21.2; LRMS (ESI) calcd for $C_{15}H_{15}NO_2[M+H]^+$: 242.11, found 242.42.



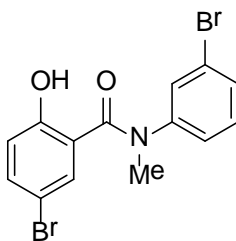
***N*-(3-bromophenyl)-2-hydroxy-*N*-methylbenzamide (3t)**

Following the general procedure I, *N*-(3-bromophenyl)-*N*-methylbenzamide (29 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFMA = 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone = 10: 1). Finally, compound (3t) (28 mg) was isolated in 92% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.44 (s, 1H), 7.32 (d, *J* = 7.56 Hz, 1H), 7.07 – 7.19 (m, 4H), 6.68 – 6.73 (m, 2H), 3.41 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.3, 155.4, 146.6, 132.0, 131.3, 131.1, 129.6, 126.8, 124.6, 122.8, 120.1, 116.7, 38.1; LRMS (ESI) calcd for C₁₄H₁₂BrNO₂[M+H]⁺: 306.01, found 306.33.



2-Hydroxy-*N*,5-dimethyl-*N*-(*m*-tolyl)benzamide (3u)

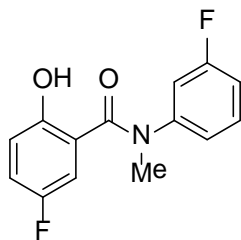
Following the general procedure I, *N*,3-dimethyl-*N*-(*m*-tolyl)benzamide (24 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFMA = 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 7 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone = 10: 1). Finally, compound (3u) (16 mg) was isolated in 63% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.12 (t, *J* = 7.72 Hz, 1H), 7.05 (s, 1H), 6.98 – 7.00 (m, 2H), 6.89 (d, *J* = 8.24 Hz, 1H), 6.81 (s, 1H), 6.59 (d, *J* = 8.28 Hz, 1H), 3.38 (s, 3H), 2.24 (s, 3H), 2.07 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.5, 153.7, 145.3, 140.1, 132.4, 129.9, 129.7, 129.0, 128.8, 128.4, 124.8, 124.0, 116.7, 38.4, 21.2, 20.3; LRMS (ESI) calcd for C₁₆H₁₇NO₂[M+H]⁺: 256.13, found 256.46.



5-Bromo-*N*-(3-bromophenyl)-2-hydroxy-*N*-methylbenzamide (3v)

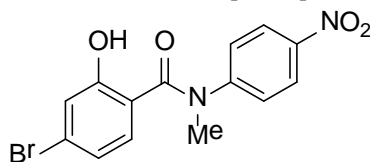
Following the general procedure I, 3-bromo-*N*-(3-bromophenyl)-*N*-methylbenzamide (37 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFMA = 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone = 10: 1). Finally, compound (3v) (30 mg) was isolated in 78% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.68 (s, 1H), 7.46 (d, *J* = 8.08 Hz, 1H), 7.33 (t, *J* = 1.80 Hz, 1H), 7.21 – 7.29 (m, 2H), 7.03 (dd, *J* = 8.00 Hz, *J* = 1.20 Hz, 1H), 6.84 (d, *J* = 8.84 Hz, 1H), 6.77 (d, *J* = 2.36 Hz, 1H), 3.47 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 170.1, 159.7, 145.9, 135.9, 132.9, 131.1, 130.9, 129.7, 125.6, 123.3, 120.0, 117.2, 109.6, 39.4; LRMS (ESI) calcd for C₁₄H₁₁Br₂NO₂[M+H]⁺: 383.92, found

384.24.



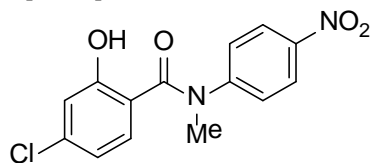
5-Fluoro-N-(3-fluorophenyl)-2-hydroxy-N-methylbenzamide (3w)

Following the general procedure I, 3-fluoro-N-(3-fluorophenyl)-N-methylbenzamide (25 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TF₂AA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 70 °C. in the sealed tube for 1.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (3w) (17 mg) was isolated in 65% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.23 – 7.29 (m, 1H), 7.04 - 7.08 (m, 2H), 6.93 – 6.97 (m, 1H), 6.84 – 6.89 (m, 2H), 6.63 – 6.67 (m, 1H), 3.41 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 170.6, 163.9 (d, *J*_{C-F}= 244 Hz), 156.9 (d, *J*_{C-F}= 236 Hz), 151.5, 146.4 (d, *J*_{C-F}= 10 Hz), 131.3 (d, *J*_{C-F}= 9 Hz), 125.6 (d, *J*_{C-F}= 7 Hz), 124.0 (d, *J*_{C-F}= 7 Hz), 118.3 (d, *J*_{C-F}= 23 Hz), 117.8 (d, *J*_{C-F}= 8 Hz), 115.7 (d, *J*_{C-F}= 24 Hz), 115.2 (d, *J*_{C-F}= 5 Hz), 115.1, 38.0; LRMS (ESI) calcd for C₁₄H₁₁F₂NO₂[M+H]⁺: 264.08, found 264.36.



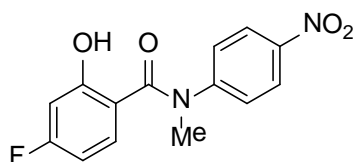
4-Bromo-2-hydroxy-N-methyl-N-(4-nitrophenyl)benzamide (3x)

Following the general procedure I, 4-bromo-N-methyl-N-(4-nitrophenyl)benzamide (34 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TF₂AA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 80 °C. in the sealed tube for 3 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (3x) (29 mg) was isolated in 82% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.12 (d, *J* = 9.04 Hz, 2H), 7.43 (d, *J* = 9.04 Hz, 2H), 7.11 (d, *J* = 8.20 Hz, 1H), 6.93 (dd, *J* = 8.20 Hz, *J* = 1.76 Hz, 1H), 6.85 (d, *J* = 1.76 Hz, 1H), 3.47 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 171.0, 156.1, 150.7, 147.2, 131.4, 128.4, 125.6, 125.1, 123.9, 123.5, 119.9, 37.8; LRMS (ESI) calcd for C₁₄H₁₁BrN₂O₄[M+H]⁺: 350.99, found 350.81.



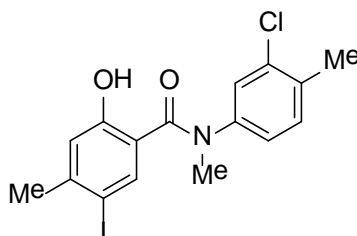
4-Chloro-2-hydroxy-N-methyl-N-(4-nitrophenyl)benzamide (3y)

Following the general procedure I, 4-chloro-N-methyl-N-(4-nitrophenyl)benzamide (29 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TF₂AA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 80 °C. in the sealed tube for 3 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (3y) (23 mg) was isolated in 75% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.67 (s, 1H), 8.20 (d, *J* = 8.64 Hz, 2H), 7.26 (d, *J* = 8.64 Hz, 2H), 6.99 (d, *J* = 1.48 Hz, 1H), 6.59 (d, *J* = 8.56 Hz, 1H), 6.46 (dd, *J* = 8.56 Hz, *J* = 1.48 Hz, 1H), 3.53 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.4, 161.6, 150.7, 145.9, 139.5, 131.2, 126.9, 125.3, 119.0, 118.7, 114.0, 39.0; LRMS (ESI) calcd for C₁₄H₁₁ClN₂O₄[M+H]⁺: 307.04, found 306.95.



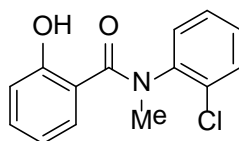
4-Fluoro-2-hydroxy-*N*-methyl-*N*-(4-nitrophenyl)benzamide (**3z**)

Following the general procedure **I**, 4-fluoro-*N*-methyl-*N*-(4-nitrophenyl)benzamide (28 mg, 0.1 mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 80 °C. in the sealed tube for 2 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3z**) (23 mg) was isolated in 78% yield. 1H -NMR (400 MHz, $CDCl_3$) δ (ppm) 10.87 (s, 1H), 8.20 (d, $J = 8.96$ Hz, 2H), 7.26 (d, $J = 8.96$ Hz, 2H), 6.64 – 6.68 (m, 2H), 6.17 – 6.22 (m, 1H), 3.53 (s, 3H); ^{13}C -NMR (100 MHz, $CDCl_3$) δ (ppm) 171.6, 165.6 (d, $J_{C-F} = 253$ Hz), 163.3 (d, $J_{C-F} = 14$ Hz), 150.9, 145.8, 132.3 (d, $J_{C-F} = 11$ Hz), 126.9, 125.3, 111.9 (d, $J_{C-F} = 3$ Hz), 106.4 (d, $J_{C-F} = 22$ Hz), 105.4 (d, $J_{C-F} = 24$ Hz), 39.1; LRMS (ESI) calcd for $C_{14}H_{11}FN_2O_4[M+H]^+$: 291.07, found 290.97.



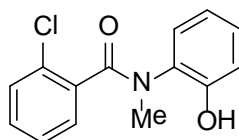
N-(3-chloro-4-methylphenyl)-2-hydroxy-5-iodo-*N*,4-dimethylbenzamide (**3a'**)

Following the general procedure **I**, *N*-(3-chloro-4-methylphenyl)-3-iodo-*N*,4-dimethylbenzamide (40 mg, 0.1 mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 70 °C. in the sealed tube for 3.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3a'**) (36 mg) was isolated in 87% yield. 1H -NMR (400 MHz, CD_3OD) δ (ppm) 7.45 (s, 1H), 7.28 (d, $J = 2.00$ Hz, 1H), 7.16 (d, $J = 8.04$ Hz, 1H), 7.02 (dd, $J = 8.04$ Hz, $J = 2.00$ Hz, 1H), 6.64 (s, 1H), 3.37 (s, 3H), 2.28 (s, 3H), 2.24 (s, 3H); ^{13}C -NMR (100 MHz, CD_3OD) δ (ppm) 170.4, 155.9, 145.3, 143.9, 139.4, 136.3, 135.1, 132.1, 128.4, 126.5, 124.4, 118.2, 87.3, 38.2, 28.1, 19.6; LRMS (ESI) calcd for $C_{16}H_{15}ClINO_2[M+H]^+$: 415.98, found 415.82.



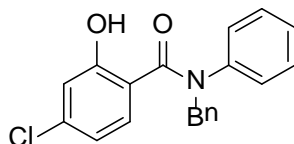
N-(2-chlorophenyl)-2-hydroxy-*N*-methylbenzamide (**3b'**)

Following the general procedure **I**, *N*-(2-chlorophenyl)-*N*-methylbenzamide (25 mg, 0.1 mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3b'**) (21 mg) was isolated in 80% yield. 1H -NMR (400 MHz, $CDCl_3$) δ (ppm) 10.65 (s, 1H), 7.44 – 7.42 (m, 1H), 7.27 – 7.15 (m, 4H), 6.92 (d, $J = 8.40$ Hz, 1H), 6.68 (s, 1H), 6.41 (s, 1H), 3.39 (s, 3H); ^{13}C -NMR (100 MHz, $CDCl_3$) δ (ppm) 172.1, 160.4, 142.6, 133.1, 132.1, 131.0, 129.8, 129.3, 129.1, 128.4, 118.0, 117.9, 116.4, 38.2; LRMS (ESI) calcd for $C_{14}H_{12}ClNO_2[M+H]^+$: 262.06, found 261.99.



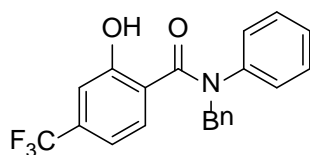
2-Chloro-*N*-(2-hydroxyphenyl)-*N*-methylbenzamide (3c')

Following the general procedure **II**, 2-chloro-*N*-methyl-*N*-phenylbenzamide (25 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFMA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 2 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (3c') (23 mg) was isolated in 88% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.29 (dd, *J* = 7.60 Hz, *J* = 1.6 Hz, 1H), 7.23 (dd, *J* = 8.00 Hz, *J* = 1.20 Hz, 1H), 7.18 – 7.11 (m, 2H), 7.06 (dt, *J* = 7.60 Hz, *J* = 1.20 Hz, 1H), 7.02 – 6.98 (m, 1H), 6.73 (dd, *J* = 8.00 Hz, *J* = 1.20 Hz, 1H), 6.61 (dt, *J* = 7.60 Hz, *J* = 1.20 Hz, 1H), 3.35 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 171.04, 154.09, 137.71, 131.55, 131.39, 131.20, 130.07, 130.02, 129.27, 128.52, 127.22, 120.55, 117.24, 36.28; LRMS (ESI) calcd for C₁₄H₁₂ClNO₂[M+H]⁺: 262.06, found 262.08.



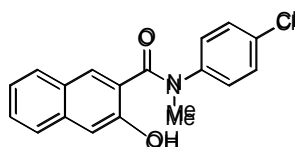
N-benzyl-4-chloro-2-hydroxy-*N*-phenylbenzamide (3d')

Following the general procedure **I**, *N*-benzyl-4-chloro-*N*-phenylbenzamide (33 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFMA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 8: 1). Finally, compound (3d') (26 mg) was isolated in 77% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 11.29 (s, 1H), 7.27 – 7.23 (m, 8H), 6.98 (d, *J* = 7.20 Hz, 2H), 6.94 (d, *J* = 1.20 Hz, 1H), 6.59 (d, *J* = 8.80 Hz, 1H), 6.35 (dd, *J* = 8.80 Hz, *J* = 1.60 Hz, 1H), 5.10 (s, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 170.70, 162.06, 143.51, 138.51, 136.68, 131.36, 129.85, 128.68, 128.58, 127.79, 127.71, 127.45, 118.34, 118.19, 114.59, 54.91; LRMS (ESI) calcd for C₂₀H₁₆ClNO₂[M+H]⁺: 338.09, found 337.94.



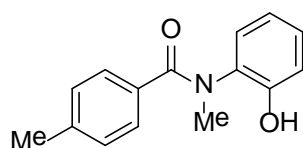
N-benzyl-2-hydroxy-*N*-phenyl-4-(trifluoromethyl)benzamide (3e')

Following the general procedure **I**, *N*-benzyl-*N*-phenyl-4-(trifluoromethyl)benzamide (36 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFMA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 8 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 8: 1). Finally, compound (3e') (25 mg) was isolated in 67% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 11.07 (s, 1H), 7.28 – 7.25 (m, 8H), 7.19 (s, 1H), 6.98 (d, *J* = 6.40 Hz, 2H), 6.78 (d, *J* = 8.32 Hz, 1H), 6.61 (d, *J* = 8.36 Hz, 1H), 5.13 (s, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 170.16, 161.00, 143.14, 136.47, 134.22 (q, *J*_{C-F}= 32 Hz), 130.91, 129.92, 128.74, 128.64, 127.96, 127.91, 127.48, 123.33 (q, *J*_{C-F}= 271 Hz), 119.20, 115.33 (q, *J*_{C-F}= 4 Hz), 114.27 (q, *J*_{C-F}= 4 Hz), 54.96; LRMS (ESI) calcd for C₂₁H₁₆F₃NO₂[M+H]⁺: 372.11, found 372.01.



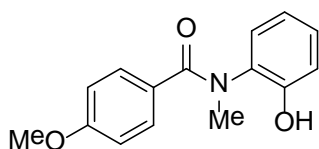
***N*-(4-chlorophenyl)-3-hydroxy-*N*-methyl-2-naphthamide (**3f'**)**

Following the general procedure **I**, *N*-(4-chlorophenyl)-*N*-methyl-2-naphthamide (30 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFSA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 2 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**3f'**) (25 mg) was isolated in 81% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.62 – 7.66 (m, 2H), 7.54 (d, *J* = 8.00 Hz, 1H), 7.34 (t, *J* = 6.00 Hz, 1H), 7.16 – 7.25 (m, 5H), 7.01 (s, 1H), 3.44 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 171.8, 152.7, 143.7, 136.5, 133.7, 129.9, 129.5, 129.5, 129.0, 128.8, 128.1, 127.9, 127.0, 124.6, 110.5, 38.1; LRMS (ESI) calcd for C₁₈H₁₄ClNO₂[M+H]⁺: 312.07, found 312.38.



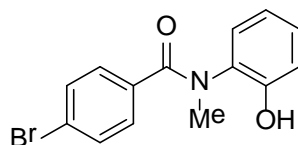
***N*-(2-hydroxyphenyl)-*N*,4-dimethylbenzamide (**4a**)**

Following the general procedure **II**, *N*,4-dimethyl-*N*-phenylbenzamide (23 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFSA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 0.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4a**) (17 mg) was isolated in 71% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.20 (d, *J* = 7.80 Hz, 2H), 7.02 (t, *J* = 7.68 Hz, 1H), 6.96 (d, *J* = 7.76 Hz, 2H), 6.90 (d, *J* = 7.68 Hz, 1H), 6.76 (d, *J* = 8.08 Hz, 1H), 6.64 (t, *J* = 7.52 Hz, 1H), 3.30 (s, 3H), 2.22 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 174.2, 154.0, 141.1, 134.6, 133.1, 130.4, 130.0, 129.2, 128.9, 120.8, 117.4, 37.3, 21.3; LRMS (ESI) calcd for C₁₅H₁₅NO₂[M+H]⁺: 242.11, found 242.42.



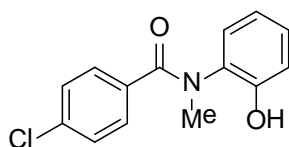
***N*-(2-hydroxyphenyl)-4-methoxy-*N*-methylbenzamide (**4b**)**

Following the general procedure **II**, 4-methoxy-*N*-methyl-*N*-phenylbenzamide (25 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFSA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 3 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4b**) (22 mg) was isolated in 86% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.28 (d, *J* = 8.44 Hz, 2H), 7.04 (t, *J* = 7.68 Hz, 1H), 6.91 (d, *J* = 7.64 Hz, 1H), 6.78 (d, *J* = 8.08 Hz, 1H), 6.66– 6.69 (m, 3H), 3.71 (s, 3H), 3.31 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 173.9, 162.3, 153.9, 133.4, 130.9, 130.3, 130.0, 129.4, 120.9, 117.5, 113.8, 55.7, 37.4; LRMS (ESI) calcd for C₁₅H₁₅NO₃[M+H]⁺: 258.11, found 258.41.



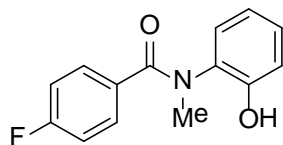
4-Bromo-*N*-(2-hydroxyphenyl)-*N*-methylbenzamide (**4c)**

Following the general procedure **II**, 4-bromo-*N*-methyl-*N*-phenylbenzamide (29 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 20 min. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4c**) (23 mg) was isolated in 75% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.32 (d, *J* = 8.36 Hz, 2H), 7.23 (t, *J* = 8.32 Hz, 2H), 7.05 (t, *J* = 7.92 Hz, 1H), 6.98 (d, *J* = 7.76 Hz, 1H), 6.77 (d, *J* = 8.12 Hz, 1H), 6.70 (t, *J* = 7.64 Hz, 1H), 3.33 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 173.0, 153.9, 136.7, 132.6, 131.8, 130.6, 130.3, 130.3, 124.8, 121.0, 117.5, 37.2; LRMS (ESI) calcd for C₁₄H₁₂BrNO₂[M+H]⁺: 306.01, found 306.33.



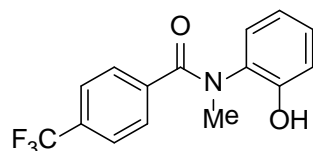
4-Chloro-*N*-(2-hydroxyphenyl)-*N*-methylbenzamide (**4d**)

Following the general procedure **II**, 4-chloro-*N*-methyl-*N*-phenylbenzamide (25 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 45 min. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4d**) (20 mg) was isolated in 77% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.30 (d, *J* = 8.36 Hz, 2H), 7.16 (d, *J* = 8.36 Hz, 2H), 7.05 (t, *J* = 7.72 Hz, 1H), 6.98 (d, *J* = 7.68 Hz, 1H), 6.77 (d, *J* = 8.08 Hz, 1H), 6.70 (t, *J* = 7.60 Hz, 1H), 3.30 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.9, 153.9, 136.6, 136.2, 132.6, 130.5, 130.3, 130.3, 128.7, 121.0, 117.5, 37.2; LRMS (ESI) calcd for C₁₄H₁₂ClNO₂[M+H]⁺: 262.06, found 262.36.



4-Fluoro-*N*-(2-hydroxyphenyl)-*N*-methylbenzamide (**4e**)

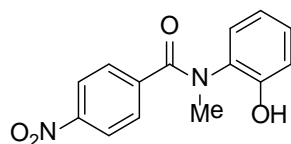
Following the general procedure **II**, 4-fluoro-*N*-methyl-*N*-phenylbenzamide (23 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 45 min. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4e**) (23 mg) was isolated in 94% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.36 (dd, *J* = 8.64 Hz, *J* = 5.48 Hz, 2H), 7.02 – 7.07 (m, 1H), 6.97 (dd, *J* = 7.80 Hz, *J* = 1.36 Hz, 1H), 6.86 – 6.91 (m, 2H), 6.77 (d, *J* = 8.16 Hz, 1H), 6.69 (t, *J* = 7.44 Hz, 1H), 3.33 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 173.0, 164.6 (d, *J*_{C-F}= 247 Hz), 153.9, 133.8, 133.8, 132.9, 131.3 (d, *J*_{C-F}= 9 Hz), 130.2 (d, *J*_{C-F}= 5 Hz), 120.9, 117.5, 115.4 (d, *J*_{C-F}= 22 Hz), 37.3; LRMS (ESI) calcd for C₁₄H₁₂FNO₂[M+H]⁺: 246.09, found 246.32.



N-(2-hydroxyphenyl)-*N*-methyl-4-(trifluoromethyl)benzamide (**4f**)

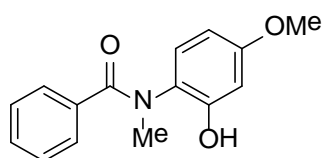
Following the general procedure **II**, *N*-methyl-*N*-phenyl-4-(trifluoromethyl)benzamide (28 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 70 °C. in the sealed tube for 0.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4f**) (22 mg) was

isolated in 75% yield. $^1\text{H-NMR}$ (400 MHz, CD_3OD) δ (ppm) 7.45 – 7.51 (m, 4H), 7.02 – 7.07 (m, 2H), 6.75 (d, $J = 8.04$ Hz, 1H), 6.70 (t, $J = 7.52$ Hz, 1H), 3.36 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CD_3OD) δ (ppm) 172.5, 153.9, 141.6, 132.3, 132.2 (q, $J_{\text{C-F}} = 33$ Hz), 130.5, 130.3, 129.3, 125.5 (q, $J_{\text{C-F}} = 4$ Hz), 125.2 (q, $J_{\text{C-F}} = 270$ Hz), 121.0, 117.5, 37.2; LRMS (ESI) calcd for $\text{C}_{15}\text{H}_{12}\text{F}_3\text{NO}_2[\text{M}+\text{H}]^+$: 296.08, found 296.34.



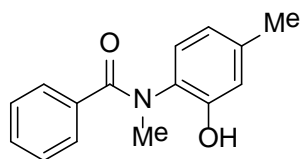
***N*-(2-hydroxyphenyl)-*N*-methyl-4-nitrobenzamide (4g)**

Following the general procedure **II**, *N*-methyl-4-nitro-*N*-phenylbenzamide (26 mg, 0.1 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (54 mg, 0.2 mmol) and $\text{Pd}(\text{OAc})_2$ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 2.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4g**) (20 mg) was isolated in 74% yield. $^1\text{H-NMR}$ (400 MHz, CD_3OD) δ (ppm) 8.03 (d, $J = 8.84$ Hz, 2H), 7.54 (d, $J = 8.84$ Hz, 2H), 7.02 – 7.07 (m, 2H), 6.70 – 6.75 (m, 2H), 3.36 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CD_3OD) δ (ppm) 171.9, 154.0, 149.5, 144.0, 132.0, 130.7, 130.3, 129.8, 123.7, 121.1, 117.5, 37.1; LRMS (ESI) calcd for $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_4[\text{M}+\text{H}]^+$: 273.08, found 273.33.



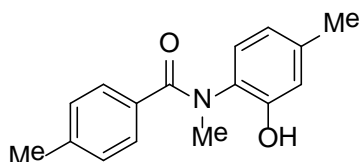
***N*-(2-hydroxy-4-methoxyphenyl)-*N*-methylbenzamide (4h)**

Following the general procedure **II**, *N*-(4-methoxyphenyl)-*N*-methylbenzamide (24 mg, 0.1 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (54 mg, 0.2 mmol) and $\text{Pd}(\text{OAc})_2$ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 50 °C. in the sealed tube for 2 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4h**) (24 mg) was isolated in 93% yield. $^1\text{H-NMR}$ (400 MHz, CD_3OD) δ (ppm) 7.34 (d, $J = 7.76$ Hz, 2H), 7.25 (t, $J = 7.16$ Hz, 1H), 7.18 (t, $J = 7.68$ Hz, 2H), 6.84 (d, $J = 8.64$ Hz, 1H), 6.34 (d, $J = 2.60$ Hz, 1H), 6.24 (dd, $J = 8.64$ Hz, $J = 2.60$ Hz, 1H), 3.67 (s, 3H), 3.32 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CD_3OD) δ (ppm) 174.4, 161.6, 154.8, 137.7, 130.8, 130.6, 128.7, 128.6, 126.2, 106.1, 102.9, 55.7, 37.4; LRMS (ESI) calcd for $\text{C}_{15}\text{H}_{15}\text{NO}_3[\text{M}+\text{H}]^+$: 258.11, found 258.41.



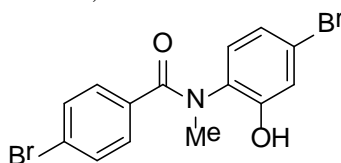
***N*-(2-hydroxy-4-methylphenyl)-*N*-methylbenzamide (4i)**

Following the general procedure **II**, *N*-methyl-*N*-(*p*-tolyl)benzamide (23 mg, 0.1 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (54 mg, 0.2 mmol) and $\text{Pd}(\text{OAc})_2$ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 50 °C. in the sealed tube for 40 min. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4i**) (18.6 mg) was isolated in 77% yield. $^1\text{H-NMR}$ (400 MHz, CD_3OD) δ (ppm) 7.32 (d, $J = 7.48$ Hz, 2H), 7.22 (t, $J = 7.32$ Hz, 1H), 7.15 (t, $J = 7.52$ Hz, 2H), 6.78 (d, $J = 7.92$ Hz, 1H), 6.59 (s, 1H), 6.46 (d, $J = 7.92$ Hz, 1H), 3.31 (s, 3H), 2.16 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CD_3OD) δ (ppm) 174.2, 153.6, 140.5, 137.7, 130.6, 130.3, 130.0, 128.7, 128.6, 121.5, 117.9, 37.3, 21.2; LRMS (ESI) calcd for $\text{C}_{15}\text{H}_{15}\text{NO}_2[\text{M}+\text{H}]^+$: 242.11, found 242.37.



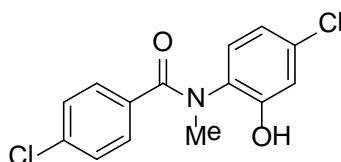
***N*-(2-hydroxy-4-methylphenyl)-*N*,4-dimethylbenzamide (**4j**)**

Following the general procedure **II**, *N*,4-dimethyl-*N*-(*p*-tolyl)benzamide (24 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 45 °C. in the sealed tube for 1 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4j**) (20 mg) was isolated in 78% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.21 (d, *J* = 7.92 Hz, 2H), 6.96 (d, *J* = 7.92 Hz, 2H), 6.76 (d, *J* = 7.92 Hz, 1H), 6.59 (s, 1H), 6.47 (d, *J* = 7.92 Hz, 1H), 3.29 (s, 3H), 2.23 (s, 3H), 2.17 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 174.3, 153.5, 141.0, 140.4, 134.6, 130.5, 129.9, 129.1, 128.9, 121.5, 117.9, 37.3, 21.3, 21.1; LRMS (ESI) calcd for C₁₆H₁₇NO₂[M+H]⁺: 256.13, found 256.36.



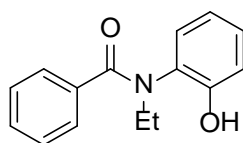
4-Bromo-*N*-(4-bromo-2-hydroxyphenyl)-*N*-methylbenzamide (**4k)**

Following the general procedure **II**, 4-bromo-*N*-(4-bromophenyl)-*N*-methylbenzamide (37 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 1 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4k**) (27 mg) was isolated in 70% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.37 (d, *J* = 8.28 Hz, 2H), 7.23 (d, *J* = 8.32 Hz, 2H), 6.93 – 6.95 (m, 2H), 6.86 (d, *J* = 8.36 Hz, 1H), 3.30 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.8, 154.9, 136.4, 132.1, 131.9, 131.7, 130.6, 125.0, 124.0, 122.9, 120.5, 37.1; LRMS (ESI) calcd for C₁₄H₁₁Br₂NO₂[M+H]⁺: 383.92, found 384.19.



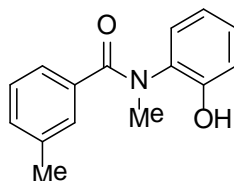
4-Chloro-*N*-(4-chloro-2-hydroxyphenyl)-*N*-methylbenzamide (**4l)**

Following the general procedure **II**, 4-chloro-*N*-(4-chlorophenyl)-*N*-methylbenzamide (28 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 80 °C. in the sealed tube for 1 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4l**) (19 mg) was isolated in 65% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.30 (d, *J* = 8.00 Hz, 2H), 7.21 (d, *J* = 8.00 Hz, 2H), 7.00 (d, *J* = 8.00 Hz, 1H), 6.78 (s, 1H), 6.72 (d, *J* = 8.00 Hz, 1H), 3.31 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.8, 154.7, 136.8, 136.0, 135.2, 131.7, 131.4, 130.4, 128.9, 120.9, 117.5, 37.2; LRMS (ESI) calcd for C₁₄H₁₁Cl₂NO₂[M+H]⁺: 296.02, found 296.34.



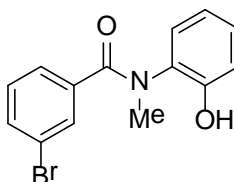
***N*-ethyl-*N*-(2-hydroxyphenyl)benzamide (**4m**)**

Following the general procedure **II**, *N*-ethyl-*N*-phenylbenzamide (23 mg, 0.1 mmol), $K_2S_2O_8$ (54 mg, 0.2 mmol) and $Pd(OAc)_2$ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 1h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4m**) (16 mg) was isolated in 66% yield. 1H -NMR (400 MHz, CD_3OD) δ (ppm) 7.32 (d, $J = 8.00$ Hz, 2H), 7.21 (t, $J = 8.00$ Hz, 1H), 7.14 (t, $J = 8.00$ Hz, 2H), 7.02 (t, $J = 8.00$ Hz, 1H), 6.91 (d, $J = 8.00$ Hz, 1H), 6.75 (d, $J = 8.00$ Hz, 1H), 6.66 (t, $J = 8.00$ Hz, 1H), 4.00 – 4.09 (m, 1H), 3.62 – 3.71(m, 1H), 1.19 (t, $J = 6.00$ Hz, 3H); ^{13}C -NMR (100 MHz, CD_3OD) δ (ppm) 173.7, 154.3, 138.0, 131.5, 131.0, 130.5, 130.1, 128.7, 128.5, 120.6, 117.4, 44.9, 12.7; LRMS (ESI) calcd for $C_{15}H_{15}NO_2[M+H]^+$: 242.11, found 242.37.



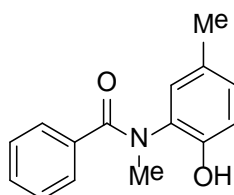
***N*-(2-hydroxyphenyl)-*N*,3-dimethylbenzamide (**4n**)**

Following the general procedure **II**, *N*,3-dimethyl-*N*-phenylbenzamide (23 mg, 0.1 mmol), $K_2S_2O_8$ (54 mg, 0.2 mmol) and $Pd(OAc)_2$ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 0.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4n**) (11 mg) was isolated in 46% yield. 1H -NMR (400 MHz, CD_3OD) δ (ppm) 7.17 (s, 1H), 7.00 – 7.10 (m, 4H), 6.91 (d, $J = 7.72$ Hz, 1H), 6.77 (d, $J = 8.12$ Hz, 1H), 6.64 (t, $J = 7.56$ Hz, 1H), 3.33 (s, 3H), 2.19 (s, 3H); ^{13}C -NMR (100 MHz, CD_3OD) δ (ppm) 174.3, 154.0, 138.5, 137.4, 133.0, 131.3, 130.4, 130.1, 129.4, 128.5, 125.9, 120.8, 117.4, 37.2, 21.2; LRMS (ESI) calcd for $C_{15}H_{15}NO_2[M+H]^+$: 242.11, found 242.47.



3-Bromo-*N*-(2-hydroxyphenyl)-*N*-methylbenzamide (4o**)**

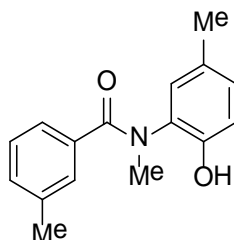
Following the general procedure **II**, 3-bromo-*N*-methyl-*N*-phenylbenzamide (29 mg, 0.1 mmol), $K_2S_2O_8$ (54 mg, 0.2 mmol) and $Pd(OAc)_2$ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 45 min. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4o**) (16 mg) was isolated in 82% yield. 1H -NMR (400 MHz, CD_3OD) δ (ppm) 7.50 (s, 1H), 7.37 (d, $J = 8.04$ Hz, 1H), 7.26 (d, $J = 7.72$ Hz, 1H), 7.03 – 7.08 (m, 2H), 6.99 (dd, $J = 7.84$ Hz, $J = 1.36$ Hz, 1H), 6.77 (dd, $J = 8.32$ Hz, $J = 1.00$ Hz, 1H), 6.69 (m, 1H), 3.33 (s, 3H); ^{13}C -NMR (100 MHz, CD_3OD) δ (ppm) 172.3, 154.0, 139.7, 133.6, 132.5, 131.7, 130.4, 130.4, 130.2, 127.4, 122.4, 121.0, 117.4, 37.2; LRMS (ESI) calcd for $C_{14}H_{12}BrNO_2[M+H]^+$: 306.01, found 306.29.



***N*-(2-hydroxy-5-methylphenyl)-*N*-methylbenzamide (**4p**)**

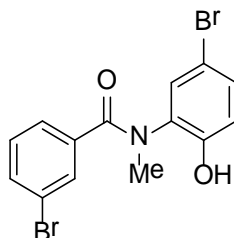
Following the general procedure **II**, *N*-methyl-*N*-(*m*-tolyl)benzamide (23 mg, 0.1 mmol), $K_2S_2O_8$ (54 mg, 0.2 mmol)

and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 0.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4p**) (20 mg) was isolated in 83% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.33 (d, *J* = 7.12 Hz, 2H), 7.23 (t, *J* = 7.32 Hz, 1H), 7.15 (t, *J* = 7.64 Hz, 2H), 6.83 (d, *J* = 8.20 Hz, 1H), 6.75 (s, 1H), 6.64 (d, *J* = 8.24 Hz, 1H), 3.32 (s, 3H), 2.08 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 174.1, 151.5, 137.6, 132.5, 130.6, 130.5, 130.4, 128.8, 128.5, 117.2, 37.3, 20.2; LRMS (ESI) calcd for C₁₅H₁₅NO₂[M+H]⁺: 242.11, found 242.66.



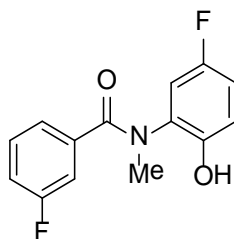
***N*-(2-hydroxy-5-methylphenyl)-*N*,3-dimethylbenzamide (**4q**)**

Following the general procedure **II**, *N*,3-dimethyl-*N*-(*m*-tolyl)benzamide (24 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 50 °C. in the sealed tube for 0.5 h, then 60 °C for 0.5 h After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4q**) (16.5 mg) was isolated in 65% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.18 (s, 1H), 7.10 (d, *J* = 7.04 Hz, 1H), 7.00 – 7.06 (m, 2H), 6.83 (dd, *J* = 8.00 Hz, *J* = 1.28 Hz, 1H), 6.74 (d, *J* = 1.76 Hz, 1H), 6.65 (d, *J* = 8.24 Hz, 1H), 6.65 (t, *J* = 7.52 Hz, 1H), 3.31 (s, 3H), 2.20 (s, 3H), 2.08 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 174.2, 151.6, 138.4, 137.5, 132.6, 131.3, 130.5, 130.5, 130.3, 129.4, 128.4, 125.9, 117.2, 37.3, 21.2, 20.2; LRMS (ESI) calcd for C₁₆H₁₇NO₂[M+H]⁺: 256.13, found 256.46.



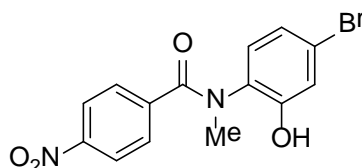
3-Bromo-*N*-(5-bromo-2-hydroxyphenyl)-*N*-methylbenzamide (**4r)**

Following the general procedure **II**, 3-bromo-*N*-(3-bromophenyl)-*N*-methylbenzamide (37 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 4 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4r**) (27 mg) was isolated in 70% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.52 (s, 1H), 7.41 (d, *J* = 7.88 Hz, 1H), 7.24 – 7.28 (m, 2H), 7.18 (d, *J* = 8.64 Hz, 1H), 7.10 (t, *J* = 7.84 Hz, 1H), 6.69 (d, *J* = 8.68 Hz, 1H), 3.31 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.1, 153.4, 139.3, 133.9, 133.8, 133.2, 133.0, 131.7, 130.5, 127.4, 122.5, 119.0, 111.6, 37.2; LRMS (ESI) calcd for C₁₄H₁₁Br₂NO₂[M+H]⁺: 383.92, found 384.24.



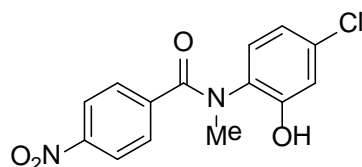
3-Fluoro-*N*-(5-fluoro-2-hydroxyphenyl)-*N*-methylbenzamide (**4s**)

Following the general procedure **II**, 3-fluoro-*N*-(3-fluorophenyl)-*N*-methylbenzamide (25 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 70 °C. in the sealed tube for 0.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4s**) (18 mg) was isolated in 68% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.18 – 7.23 (m, 1H), 7.14 (d, *J* = 7.48 Hz, 1H), 7.09 (d, *J* = 9.20 Hz, 1H), 7.01 (t, *J* = 8.24 Hz, 1H), 6.81 – 6.88 (m, 2H), 6.72 – 6.75 (m, 1H), 3.32 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.4, 163.3 (d, *J*_{C-F}= 244 Hz), 157.0 (d, *J*_{C-F}= 236 Hz), 150.5 (d, *J*_{C-F}= 3 Hz), 139.6 (d, *J*_{C-F}= 7 Hz), 132.9, 130.7 (d, *J*_{C-F}= 8 Hz), 124.6, 118.0 (d, *J*_{C-F}= 9 Hz), 117.6 (d, *J*_{C-F}= 22 Hz), 116.8 (d, *J*_{C-F}= 24 Hz), 116.7 (d, *J*_{C-F}= 23 Hz), 115.6 (d, *J*_{C-F}= 24 Hz), 37.0; LRMS (ESI) calcd for C₁₄H₁₁F₂NO₂[M+H]⁺: 264.08, found 264.36.



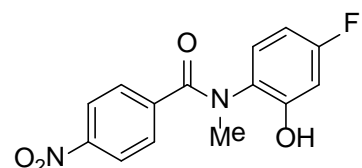
N-(4-bromo-2-hydroxyphenyl)-*N*-methyl-4-nitrobenzamide (**4t**)

Following the general procedure **II**, *N*-(4-bromophenyl)-*N*-methyl-4-nitrobenzamide (34 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 70 °C. in the sealed tube for 3 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4t**) (32.5 mg) was isolated in 93% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.07 (d, *J* = 8.80 Hz, 2H), 7.54 (d, *J* = 8.80 Hz, 2H), 7.03 (d, *J* = 8.40 Hz, 1H), 6.91 (d, *J* = 1.60 Hz, 1H), 6.86 (dd, *J* = 8.40 Hz, *J* = 1.60 Hz, 1H), 3.34 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 171.8, 155.0, 149.6, 143.7, 131.8, 131.6, 129.8, 124.1, 123.9, 123.3, 120.6, 37.0; LRMS (ESI) calcd for C₁₄H₁₁BrN₂O₄[M+H]⁺: 350.99, found 350.81.



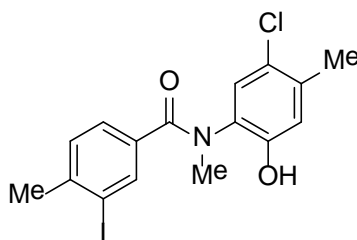
N-(4-chloro-2-hydroxyphenyl)-*N*-methyl-4-nitrobenzamide (**4u**)

Following the general procedure **II**, *N*-(4-chlorophenyl)-*N*-methyl-4-nitrobenzamide (29 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 80 °C. in the sealed tube for 1.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4u**) (22 mg) was isolated in 72% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.07 (d, *J* = 8.40 Hz, 2H), 7.54 (d, *J* = 8.40 Hz, 2H), 7.09 (d, *J* = 8.40 Hz, 1H), 6.75 (d, *J* = 2.00 Hz, 1H), 6.71 (dd, *J* = 8.40 Hz, *J* = 2.00 Hz, 1H), 3.34 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 171.8, 154.8, 149.6, 143.7, 135.6, 131.5, 131.1, 129.8, 123.9, 121.1, 117.5, 37.0; LRMS (ESI) calcd for C₁₄H₁₁ClN₂O₄[M+H]⁺: 307.04, found 306.90.



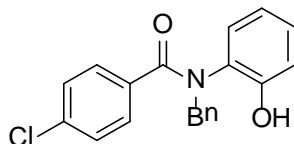
***N*-(4-fluoro-2-hydroxyphenyl)-*N*-methyl-4-nitrobenzamide (4v)**

Following the general procedure **II**, *N*-(4-fluorophenyl)-*N*-methyl-4-nitrobenzamide (28 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 80 °C. in the sealed tube for 2.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4v**) (24 mg) was isolated in 83% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.06 (d, *J* = 8.40 Hz, 2H), 7.54 (d, *J* = 8.80 Hz, 2H), 7.09 – 7.13 (m, 1H), 6.43 – 6.49 (m, 2H), 3.34 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.0, 164.1 (d, *J*_{C-F}= 245 Hz), 155.4 (d, *J*_{C-F}= 12 Hz), 149.5, 143.9, 131.6 (d, *J*_{C-F}= 11 Hz), 129.7, 128.6 (d, *J*_{C-F}= 3 Hz), 123.8, 107.6 (d, *J*_{C-F}= 23 Hz), 104.5 (d, *J*_{C-F}= 25 Hz), 37.2; LRMS (ESI) calcd for C₁₄H₁₁FN₂O₄[M+H]⁺: 291.07, found 290.58.



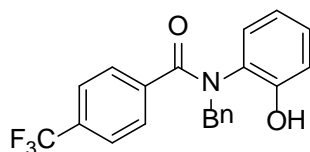
***N*-(5-chloro-2-hydroxy-4-methylphenyl)-3-iodo-*N*,4-dimethylbenzamide (4w)**

Following the general procedure **II**, *N*-(3-chloro-4-methylphenyl)-3-iodo-*N*,4-dimethylbenzamide (40 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 2 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4w**) (26 mg) was isolated in 62% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.81 (d, *J* = 1.08 Hz, 1H), 7.22 (dd, *J* = 7.84 Hz, *J* = 1.08 Hz, 1H), 7.10 (d, *J* = 7.84 Hz, 1H), 7.05 (s, 1H), 6.69 (s, 1H), 3.28 (s, 3H), 2.32 (s, 3H), 2.21 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.1, 152.7, 144.5, 139.4, 138.2, 136.5, 131.5, 130.1, 129.8, 128.7, 124.9, 119.4, 100.2, 37.3, 28.1, 19.9; LRMS (ESI) calcd for C₁₆H₁₅ClINO₂[M+H]⁺: 415.98, found 415.82.



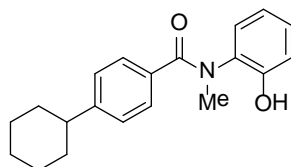
***N*-benzyl-4-chloro-*N*-(2-hydroxyphenyl)benzamide (4x)**

Following the general procedure **II**, *N*-benzyl-4-chloro-*N*-phenylbenzamide (33 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 3 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4x**) (21 mg) was isolated in 63% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.33 (d, *J* = 8.40 Hz, 2H), 7.29– 7.21 (m, 5H), 7.16 (d, *J* = 8.40 Hz, 2H), 6.99 (dt, *J* = 8.00 Hz, *J* = 1.60 Hz, 1H), 6.74 (dd, *J* = 8.00 Hz, *J* = 0.80 Hz, 1H), 6.57 (dd, *J* = 7.60 Hz, *J* = 1.60 Hz, 1H), 6.51 (dt, *J* = 7.60 Hz, *J* = 1.20 Hz, 1H), 5.51 (d, *J* = 14.40 Hz, 1H), 4.51 (d, *J* = 14.40 Hz, 1H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.73, 154.01, 138.52, 136.59, 136.40, 131.56, 130.61, 130.45, 130.26, 130.03, 129.28, 128.78, 128.45, 120.43, 117.39, 53.07; LRMS (ESI) calcd for C₂₀H₁₆ClNO₂[M+H]⁺: 338.09, found 337.94.



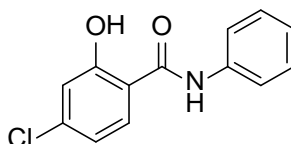
***N*-benzyl-*N*-(2-hydroxyphenyl)-4-(trifluoromethyl)benzamide (4y)**

Following the general procedure **II**, *N*-benzyl-*N*-phenyl-4-(trifluoromethyl)benzamide (36 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFMA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 2 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4y**) (24 mg) was isolated in 65% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.53 (d, *J* = 8.40 Hz, 2H), 7.46 (d, *J* = 8.40 Hz, 2H), 7.32–7.22 (m, 5H), 6.98 (dt, *J* = 7.80 Hz, *J* = 1.60 Hz, 1H), 6.73 (dd, *J* = 8.00 Hz, *J* = 1.20 Hz, 1H), 6.62 (dd, *J* = 7.60 Hz, *J* = 1.60 Hz, 1H), 6.51 (dt, *J* = 7.60 Hz, *J* = 1.20 Hz, 1H), 5.53 (d, *J* = 14.40 Hz, 1H), 4.54 (d, *J* = 14.40 Hz, 1H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.40, 154.05, 141.68, 138.37, 132.17 (q, *J*_{C-F} = 32 Hz), 131.54, 130.46, 130.25, 130.06, 129.32, 129.30, 128.51, 125.55 (q, *J*_{C-F} = 4 Hz), 125.21 (q, *J*_{C-F} = 270 Hz), 120.44, 117.38, 53.07; LRMS (ESI) calcd for C₂₁H₁₆F₃NO₂[M+H]⁺: 372.11, found 372.10.



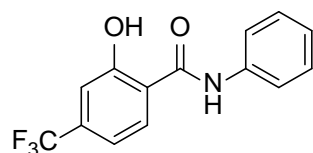
4-Cyclohexyl-*N*-(2-hydroxyphenyl)-*N*-methylbenzamide (4z)

Following the general procedure **II**, 4-cyclohexyl-*N*-methyl-*N*-phenylbenzamide (30 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFMA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 0.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**4z**) (16 mg) was isolated in 52% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.25 (d, *J* = 8.04 Hz, 2H), 6.99 – 7.05 (m, 3H), 6.91 (d, *J* = 7.52 Hz, 1H), 6.78 (d, *J* = 8.04 Hz, 1H), 6.66 (t, *J* = 7.48 Hz, 1H), 3.32 (s, 3H), 2.39 – 2.44 (m, 1H), 1.74 – 1.80 (m, 5H), 1.22 – 1.42 (m, 5H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 174.1, 154.0, 151.2, 134.9, 133.1, 130.4, 130.0, 129.1, 127.0, 120.9, 117.5, 45.7, 37.4, 35.4, 27.9, 27.1; LRMS (ESI) calcd for C₂₀H₂₃NO₂[M+H]⁺: 310.17, found 310.48.



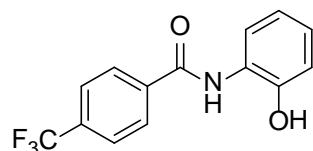
4-Chloro-2-hydroxy-*N*-phenylbenzamide (5a)

A mixture of *N*-benzyl-4-chloro-2-hydroxy-*N*-phenylbenzamide (34 mg, 0.1 mmol), EtOH (0.4 ml), AcOH (0.4 ml) in 4 ml HBr (48 wt.% in water) was stirred in a 25 ml round bottom flask for 11 h at 90 °C under an argon atmosphere. The product mixture was cooled to room temperature, dichloromethane was added to dilute the reaction mixture and saturated aqueous NaHCO₃ was added to neutralize acid. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 4: 1). Finally, compound (**5a**) (17.5 mg) was isolated in 71% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.94 (d, *J* = 8.40 Hz, 1H), 7.65 (d, *J* = 7.60 Hz, 2H), 7.37 (t, *J* = 7.60 Hz, 2H), 7.16 (t, *J* = 7.20 Hz, 1H), 6.99 (d, *J* = 2.00 Hz, 1H), 6.97 (dd, *J* = 8.80 Hz, *J* = 2.00 Hz, 1H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 168.04, 161.42, 140.27, 139.08, 131.27, 129.88, 125.90, 122.57, 120.65, 118.33, 117.13; LRMS (ESI) calcd for C₁₃H₁₀ClNO₂[M+H]⁺: 248.04, found 248.10.



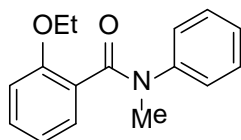
2-Hydroxy-*N*-phenyl-4-(trifluoromethyl)benzamide (**5b**)

N-benzyl-2-hydroxy-*N*-phenyl-4-(trifluoromethyl)benzamide (38 mg, 0.1 mmol), Pd/C, and AcOH (1 ml) were placed in a round bottom flask (25 ml). The flask was purged with H₂ three times to remove air, and the reaction mixture was stirred with a balloon of H₂ at 70 °C for 4 h. The product mixture was cooled to room temperature, dichloromethane was added to dilute the reaction mixture and saturated aqueous NaHCO₃ was added to neutralize acid. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 4: 1). Finally, compound (**5b**) (22 mg) was isolated in 78% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.11 (d, *J* = 8.68 Hz, 1H), 7.67 (d, *J* = 8.12 Hz, 2H), 7.37 (t, *J* = 7.84 Hz, 2H), 7.23–7.22 (m, 2H), 7.17 (t, *J* = 7.28 Hz, 1H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 167.41, 160.34, 138.99, 135.95 (q, *J*_{C-F} = 33 Hz), 131.21, 129.91, 126.04, 124.92 (q, *J*_{C-F} = 270 Hz), 122.51, 121.99, 116.61 (q, *J*_{C-F} = 4 Hz), 115.22 (q, *J*_{C-F} = 4 Hz); LRMS (ESI) calcd for C₁₄H₁₀F₃NO₂[M+H]⁺: 282.07, found 282.30.



N-(2-hydroxyphenyl)-4-(trifluoromethyl)benzamide (**5c**)

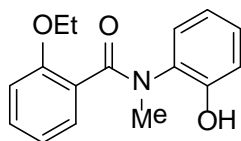
N-benzyl-*N*-(2-hydroxyphenyl)-4-(trifluoromethyl)benzamide (38 mg, 0.1 mmol), Pd/C, and AcOH (1 ml) were placed in a round bottom flask (25 ml). The flask was purged with H₂ three times to remove air, and the reaction mixture was stirred with a balloon of H₂ at 70 °C for 4 h. The product mixture was cooled to room temperature, dichloromethane was added to dilute the reaction mixture and saturated aqueous NaHCO₃ was added to neutralize acid. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 4: 1). Finally, compound (**5c**) (17.5 mg) was isolated in 63% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.10 (d, *J* = 8.00 Hz, 2H), 7.81–7.79 (m, 3H), 7.08–7.04 (m, 1H), 6.92 (dd, *J* = 8.00 Hz, *J* = 1.20 Hz, 1H), 6.87 (dt, *J* = 8.00 Hz, *J* = 1.20 Hz, 1H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 166.98, 150.29, 139.47, 134.26 (q, *J*_{C-F} = 32 Hz), 129.28, 127.33, 126.73, 126.65 (q, *J*_{C-F} = 4 Hz), 125.26 (q, *J*_{C-F} = 270 Hz), 124.45, 120.73, 116.94; LRMS (ESI) calcd for C₁₄H₁₀F₃NO₂[M+H]⁺: 282.07, found 282.01.



2-Ethoxy-*N*-methyl-*N*-phenylbenzamide (**6a**)

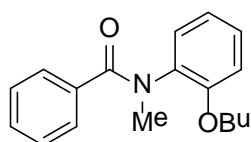
A mixture of 2-hydroxy-*N*-methyl-*N*-phenylbenzamide (171 mg, 0.75 mmol) and t-BuOK (3 mmol) in THF (7 ml) was stirred in a round bottom flask (50 ml) at room temperature for 15 min. Then, EtI (3 mmol) was added slowly. The reaction mixture was stirred for 6 h at room temperature. The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO₃, extracted by DCM. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 4: 1). Finally, compound (**6a**) (151 mg) was isolated in 79% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 7.18–7.05 (m, 7H), 6.78 (m, 1H), 6.59 (d, *J* = 6.80 Hz, 1H), 3.84 (m,

2H), 3.49 (s, 3H), 1.37 (m, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 169.47, 154.53, 144.08, 130.24, 128.84, 128.43, 127.00, 126.77, 126.58, 120.15, 111.50, 63.52, 37.16, 14.89; LRMS (ESI) calcd for $\text{C}_{16}\text{H}_{17}\text{NO}_2[\text{M}+\text{H}]^+$: 256.13, found 256.19.



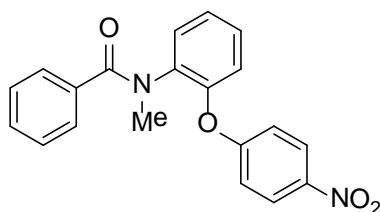
2-Ethoxy-*N*-(2-hydroxyphenyl)-*N*-methylbenzamide (6b)

Following the general procedure II, 2-ethoxy-*N*-methyl-*N*-phenylbenzamide (26 mg, 0.1 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (68 mg, 0.25 mmol) and $\text{Pd}(\text{OAc})_2$ (15 mol%, 0.015 mmol) were used with TFA: TFAA = 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 1.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone = 4: 1). Finally, compound (6b) (15 mg) was isolated in 56% yield. $^1\text{H-NMR}$ (400 MHz, CD_3OD) δ (ppm) 7.18 – 7.10 (m, 2H), 7.02 (d, $J = 7.72$ Hz, 1H), 6.96 (t, $J = 7.28$ Hz, 1H), 6.76 – 6.68 (m, 3H), 6.57 (t, $J = 7.64$ Hz, 1H), 3.98 (q, $J = 6.92$ Hz, 2H), 3.32 (s, 3H), 1.43 (t, $J = 6.96$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CD_3OD) δ (ppm) 172.67, 156.00, 154.00, 131.82, 131.30, 130.21, 129.58, 128.32, 127.94, 120.64, 120.12, 117.08, 112.46, 64.70, 36.24, 15.07; LRMS (ESI) calcd for $\text{C}_{16}\text{H}_{17}\text{NO}_3[\text{M}+\text{H}]^+$: 272.12, found 272.17.



N-(2-butoxyphenyl)-*N*-methylbenzamide (6c)

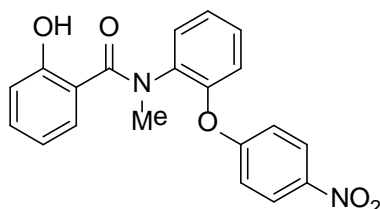
A mixture of *N*-(2-hydroxyphenyl)-*N*-methylbenzamide (227 mg, 1 mmol) and *t*-BuOK (8 mmol) in THF (7 ml) was stirred in a round bottom flask (50 ml) at room temperature for 15 min. Then, BuI (8 mmol) was added slowly. The reaction mixture was stirred for 16 h at room temperature. The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO_3 , extracted by DCM. The organic layer was dried over anhydrous Na_2SO_4 , and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate = 10: 1). Finally, compound (6c) (170 mg) was isolated in 60% yield. $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 7.30 (d, $J = 7.20$ Hz, 2H), 7.17 – 7.09 (m, 4H), 6.96 (d, $J = 5.60$ Hz, 1H), 6.79 – 6.72 (m, 2H), 3.94 – 3.85 (m, 2H), 3.35 (s, 3H), 1.82 – 1.74 (m, 2H), 1.54 – 1.47 (m, 2H), 0.98 (t, $J = 7.20$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 171.55, 154.11, 136.43, 133.57, 129.49, 129.41, 128.67, 127.99, 127.46, 120.53, 112.33, 67.80, 37.08, 31.36, 19.38, 13.90; LRMS (ESI) calcd for $\text{C}_{18}\text{H}_{21}\text{NO}_2[\text{M}+\text{H}]^+$: 284.16, found 283.81.



N-methyl-*N*-(2-(4-nitrophenoxy)phenyl)benzamide (6d)

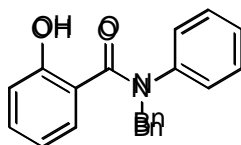
A mixture of *N*-(2-hydroxyphenyl)-*N*-methylbenzamide (68 mg, 0.3 mmol), 1-fluoro-4-nitrobenzene (47 mg, 0.33 mmol), K_2CO_3 (207 mg, 1.5 mmol) in DMF (0.5 ml) was stirred in a round bottom flask (25 ml) at 50 °C for 5 h. The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO_3 , extracted by DCM. The organic layer was dried over anhydrous Na_2SO_4 , and evaporated in vacuum to afford the crude

product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 4: 1). Finally, compound (**6d**) (88 mg) was isolated in 84% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 8.12 (d, *J* = 8.72 Hz, 2H), 7.40 (d, *J* = 6.48 Hz, 1H), 7.29 (d, *J* = 7.60 Hz, 2H), 7.25 – 7.13 (m, 5H), 6.87 – 6.77 (m, 3H), 3.34 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 170.89, 161.67, 150.04, 143.17, 136.54, 135.53, 129.89, 129.78, 128.82, 128.30, 127.68, 125.83, 125.79, 120.56, 117.42, 38.06; LRMS (ESI) calcd for C₂₀H₁₆N₂O₄[M+H]⁺: 349.11, found 349.20.



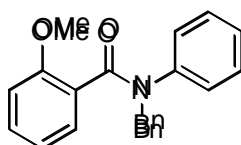
2-Hydroxy-*N*-methyl-*N*-(2-(4-nitrophenoxy)phenyl)benzamide (**6e**)

Following the general procedure **I**, *N*-methyl-*N*-(2-(4-nitrophenoxy)phenyl)benzamide (70 mg, 0.2 mmol), K₂S₂O₈ (162 mg, 0.6 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.01 mmol) were used with TFA: TFAA= 1.8 ml: 0.2 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**6e**) (46 mg) was isolated in 63% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.33 (s, 1H), 8.07 (d, *J* = 9.16 Hz, 2H), 7.52 – 7.50 (m, 1H), 7.33 – 7.26 (m, 2H), 7.17 (dt, *J* = 7.76 Hz, *J* = 1.24 Hz, 1H), 6.91 – 6.86 (m, 2H), 6.77 (d, *J* = 8.28 Hz, 1H), 6.68 (d, *J* = 9.12 Hz, 2H), 6.46 (t, *J* = 7.52 Hz, 1H), 3.34 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 172.62, 161.47, 160.22, 149.79, 143.33, 137.16, 133.01, 129.16, 129.12, 129.09, 126.39, 125.92, 121.07, 117.98, 117.82, 117.33, 116.77, 38.78; LRMS (ESI) calcd for C₂₀H₁₆N₂O₅[M+H]⁺: 365.11, found 365.13.



N-benzyl-2-hydroxy-*N*-phenylbenzamide (**6f**)

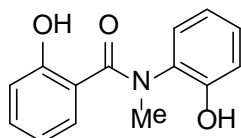
Following the general procedure **I**, *N*-benzyl-*N*-phenylbenzamide (29 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 10: 1). Finally, compound (**6f**) (29 mg) was isolated in 96% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.72 (s, 1H), 7.22 – 7.06 (m, 9H), 6.92 (d, *J* = 7.60 Hz, 2H), 6.85 (d, *J* = 8.40 Hz, 1H), 6.64 (d, *J* = 8.00 Hz, 1H), 6.30 (t, *J* = 7.60 Hz, 1H), 5.05 (s, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.44, 160.90, 143.88, 136.94, 132.94, 130.44, 129.63, 128.65, 128.47, 127.68, 127.42, 127.39, 117.97, 117.87, 116.27, 54.79; LRMS (ESI) calcd for C₂₀H₁₇NO₂[M+H]⁺: 304.13, found 304.42.



N-benzyl-2-methoxy-*N*-phenylbenzamide (**6g**)

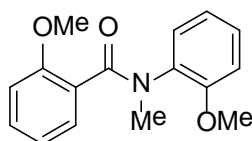
A mixture of *N*-benzyl-2-hydroxy-*N*-phenylbenzamide (31 mg, 0.1 mmol) and *t*-BuOK (0.3 mmol) in THF (0.6 ml) was stirred in a round bottom flask (25 ml) at room temperature for 15 min. Then, MeI (0.3 mmol) was added slowly. The reaction mixture was stirred for 12 h at room temperature. The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO₃, extracted by DCM. The organic layer was dried over

anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 4: 1). Finally, compound (**6g**) (28 mg) was isolated in 89% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 7.29 – 7.13 (m, 6H), 7.05 (t, *J* = 7.52 Hz, 1H), 6.96 – 6.94 (m, 3H), 6.82 (d, *J* = 6.52 Hz, 2H), 6.71 (t, *J* = 7.32 Hz, 1H), 6.53 (d, *J* = 8.24 Hz, 1H), 5.05 (s, 2H), 3.56 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 169.28, 155.13, 142.60, 137.75, 130.33, 128.72, 128.47, 128.44, 128.29, 127.76, 127.29, 126.91, 126.77, 120.28, 110.62, 55.20, 52.96; LRMS (ESI) calcd for C₂₁H₁₉NO₂[M+H]⁺: 318.14, found 318.21.



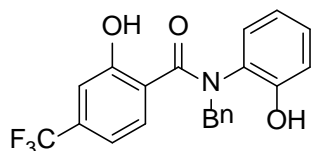
2-Hydroxy-*N*-(2-hydroxyphenyl)-*N*-methylbenzamide (**6h**)

Following the general procedure **II**, 2-hydroxy-*N*-methyl-*N*-phenylbenzamide (23 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (15 mol%, 0.015 mmol) were used with TFA: TFSA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 1 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**6h**) (14.5 mg) was isolated in 60% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.07 – 7.01 (m, 4H), 6.75 (d, *J* = 7.60 Hz, 1H), 6.68 – 6.61 (m, 2H), 6.51 (t, *J* = 6.80 Hz, 1H), 3.31 (s, 3H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 173.21, 156.52, 153.83, 132.54, 131.85, 130.14, 129.58, 128.86, 123.74, 120.60, 119.31, 117.27, 116.79, 36.80; LRMS (ESI) calcd for C₁₄H₁₃NO₃[M+H]⁺: 244.09, found 244.11.



2-Methoxy-*N*-(2-methoxyphenyl)-*N*-methylbenzamide (**6i**)

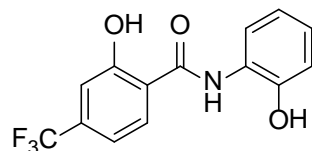
A mixture of 2-hydroxy-*N*-(2-hydroxyphenyl)-*N*-methylbenzamide (25 mg, 0.1 mmol) and t-BuOK (0.4 mmol) in THF (1 ml) was stirred in a round bottom flask (25 ml) at room temperature for 15 min. Then, MeI (0.4 mmol) was added slowly. The reaction mixture was stirred for 12 h at room temperature. The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO₃, extracted by DCM. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 4: 1). Finally, compound (**6i**) (19 mg) was isolated in 70% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 7.14 (dd, *J* = 7.60 Hz, *J* = 1.60 Hz, 1H), 7.10 – 7.05 (m, 3H), 6.71 – 6.66 (m, 3H), 6.60 (d, *J* = 8.40 Hz, 1H), 3.76 (s, 3H), 3.68 (s, 3H), 3.35 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 169.80, 155.28, 154.69, 132.43, 130.02, 128.84, 128.80, 127.77, 126.84, 120.03, 119.76, 111.10, 110.31, 55.22, 55.19, 35.95; LRMS (ESI) calcd for C₁₆H₁₇NO₃[M+H]⁺: 272.12, found 272.07.



N-benzyl-2-hydroxy-*N*-(2-hydroxyphenyl)-4-(trifluoromethyl)benzamide (**6j**)

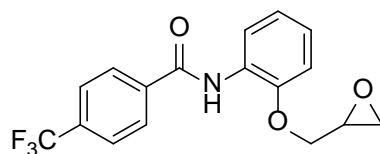
Following the general procedure **II**, *N*-benzyl-2-hydroxy-*N*-phenyl-4-(trifluoromethyl)benzamide (38 mg, 0.1 mmol), K₂S₂O₈ (68 mg, 0.25 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFSA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C. in the sealed tube for 2 h. After completion of the reaction, the residue was purified by silica gel column chromatography (n-hexane: acetone= 4: 1). Finally, compound (**6j**)

(26 mg) was isolated in 67% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 7.35 (d, *J* = 7.12 Hz, 2H), 7.30–7.20 (m, 4H), 6.95 (dt, *J* = 7.48 Hz, *J* = 1.32 Hz, 1H), 6.90 (s, 1H), 6.85 (d, *J* = 7.96 Hz, 1H), 6.77 (dd, *J* = 7.80 Hz, *J* = 1.20 Hz, 1H), 6.71 (d, *J* = 8.08 Hz, 1H), 6.44 (t, *J* = 7.48 Hz, 1H), 5.65 (d, *J* = 14.56 Hz, 1H), 4.39 (d, *J* = 14.56 Hz, 1H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 171.59, 155.86, 154.03, 138.34, 133.08 (q, *J*_{C-F} = 32 Hz), 130.78, 130.54, 129.82, 129.74, 129.24, 129.18, 129.04, 128.36, 125.07 (q, *J*_{C-F} = 270 Hz), 119.94, 117.04, 115.95 (q, *J*_{C-F} = 4 Hz), 113.02 (q, *J*_{C-F} = 4 Hz), 52.37; LRMS (ESI) calcd for C₂₁H₁₆F₃NO₃[M+H]⁺: 388.11, found 388.09.



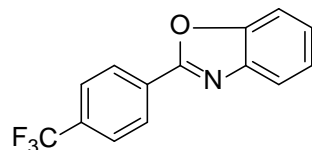
2-Hydroxy-*N*-(2-hydroxyphenyl)-4-(trifluoromethyl)benzamide (**6k**)

N-benzyl-2-hydroxy-*N*-(2-hydroxyphenyl)-4-(trifluoromethyl)benzamide (39 mg, 0.1 mmol), Pd/C, and AcOH (1 ml) were placed in a round bottom flask (25 ml). The flask was purged with H₂ three times to remove air, and the reaction mixture was stirred with a balloon of H₂ at 70 °C for 4 h. The product mixture was cooled to room temperature, dichloromethane was added to dilute the reaction mixture and saturated aqueous NaHCO₃ was added to neutralize acid. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 4: 1). Finally, compound (**6k**) (15.5 mg) was isolated in 52% yield. ¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.23–8.20 (m, 2H), 7.26 (d, *J* = 8.40 Hz, 1H), 7.24 (s, 1H), 7.01–6.97 (m, 1H), 6.90–6.84 (m, 2H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 165.10, 158.58, 148.87, 135.68 (q, *J*_{C-F} = 32 Hz), 132.77, 127.61, 126.07, 124.98 (q, *J*_{C-F} = 270 Hz), 123.33, 122.66, 120.63, 117.05 (q, *J*_{C-F} = 4 Hz), 115.88, 114.75 (q, *J*_{C-F} = 4 Hz); LRMS (ESI) calcd for C₁₄H₁₀F₃NO₃[M+H]⁺: 298.06, found 298.04.



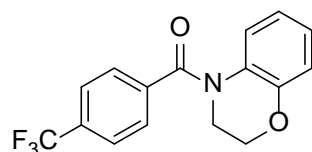
N-(2-(oxiran-2-ylmethoxy)phenyl)-4-(trifluoromethyl)benzamide (**6l**)

A mixture of *N*-(2-hydroxyphenyl)-4-(trifluoromethyl)benzamide (40 mg, 0.14 mmol) and Cs₂CO₃ (0.42 mmol) in CH₃CN (1.2 ml) was stirred in a round bottom flask (25 ml) at room temperature for 20 min. Then, 1-bromo-2,3-epoxypropane (0.56 mmol) was added slowly. The reaction mixture was stirred for 10 h at room temperature. The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO₃, extracted by DCM. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 4: 1). Finally, compound (**6l**) (36.5 mg) was isolated in 77% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 8.09 (d, *J* = 8.40 Hz, 2H), 8.05 (d, *J* = 8.00 Hz, 1H), 7.79 (d, *J* = 8.00 Hz, 2H), 7.16 (dt, *J* = 7.80 Hz, *J* = 1.20 Hz, 1H), 7.07–7.00 (m, 2H), 4.45 (dd, *J* = 11.20 Hz, *J* = 2.00 Hz, 1H), 3.98 (dd, *J* = 11.60 Hz, *J* = 6.00 Hz, 1H), 3.42–3.38 (m, 1H), 2.91 (t, *J* = 4.40 Hz, 1H), 2.80 (dd, *J* = 4.80 Hz, *J* = 2.80 Hz, 1H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 164.81, 149.02, 137.68, 132.60 (q, *J*_{C-F} = 32 Hz), 127.32, 126.54, 125.16, 124.92 (q, *J*_{C-F} = 4 Hz), 123.25 (q, *J*_{C-F} = 270 Hz), 122.24, 120.86, 112.29, 69.15, 49.50, 43.52; LRMS (ESI) calcd for C₁₇H₁₄F₃NO₃[M+H]⁺: 338.09, found 338.09.



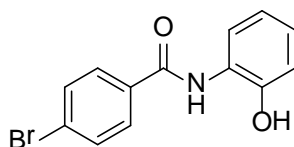
2-(4-(Trifluoromethyl)phenyl)benzo[d]oxazole (**6m**)

N-(2-hydroxyphenyl)-4-(trifluoromethyl)benzamide (36.5 mg, 0.13 mmol), *p*-toluenesulfonic acid monohydrate (80 mg, 0.42 mmol) and toluene (1 ml) were placed in a round bottom flask (25 ml). The flask was purged with Ar three times to remove air, and the reaction mixture was stirred with a balloon of Ar at 110 °C for 3 h. The product mixture was cooled to room temperature. The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO₃, extracted by DCM. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 15: 1). Finally, compound (**6m**) (20.5 mg) was isolated in 60% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 8.37 (d, *J* = 8.00 Hz, 2H), 7.83 – 7.78 (m, 3H), 7.63 – 7.59 (m, 1H), 7.43 – 7.37 (m, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 161.62, 151.01, 142.05, 133.14 (q, *J*_{C-F}= 32 Hz), 130.59, 128.00, 126.07 (q, *J*_{C-F}= 4 Hz), 125.96, 125.09, 123.90 (q, *J*_{C-F}= 271 Hz), 120.56, 110.95; LRMS (ESI) calcd for C₁₄H₈F₃NO[M+H]⁺: 264.06, found 264.42.



(2*H*-benzo[*b*][1,4]oxazin-4(3*H*)-yl)(4-(trifluoromethyl)phenyl)methanonede (**6n)**

To a 25 mL round bottom flask, *N*-(2-hydroxyphenyl)-4-(trifluoromethyl)benzamide (54 mg, 0.19 mmol), K₂CO₃ (3.8 mmol), acetone (4 ml) were added, then 1,2-dibromoethane (1.52 mmol) was added. The reaction mixture was stirred for 5 h at 60 °C (under reflux). The reaction was quenched by water and the mixture was washed once with saturated aqueous NaHCO₃, extracted by DCM. The organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum to afford the crude product, which was further purified by silica gel column chromatography (petroleum ether: ethyl acetate= 10: 1). Finally, compound (**6n**) (37.5 mg) was isolated in 64% yield. ¹H-NMR (400 MHz, CDCl₃) δ (ppm) 7.65 – 7.60 (m, 4H), 7.01 (dt, *J* = 7.80 Hz, *J* = 1.20 Hz, 1H), 6.92 (dd, *J* = 8.00 Hz, *J* = 1.20 Hz, 1H), 6.66 (t, *J* = 7.20 Hz, 1H), 4.39 (t, *J* = 4.40 Hz, 2H), 4.01 (t, *J* = 4.40 Hz, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 167.35, 146.40, 138.86, 132.51 (q, *J*_{C-F}= 33 Hz), 129.02, 126.29, 125.62 (q, *J*_{C-F}= 4 Hz), 124.47, 123.73 (q, *J*_{C-F}= 271 Hz), 120.18, 117.56, 66.56, 42.43; LRMS (ESI) calcd for C₁₆H₁₂F₃NO₂[M+H]⁺: 308.08, found 308.07.

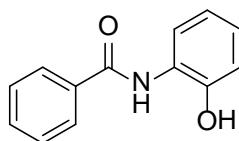


4-Bromo-*N*-(2-hydroxyphenyl)benzamide (**7a)**

1)Following the general procedure **I**, 4-bromo-*N*-phenylbenzamide (30 mg, 0.1mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 50 °C in the sealed tube for 4 h. After completion of the reaction, the residue was purified by silica gel column chromatography (Petroleum ether: Ethylacetate= 10: 1). Finally, compound (**7a**) (9.1 mg) was isolated in 31% yield.

2)Following the general procedure **II**, 4-bromo-*N*-phenylbenzamide (30 mg, 0.1mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 50 °C. in the sealed tube for 4 h. After completion of the reaction, the residue was purified by silica gel column chromatography (Petroleum ether: Ethylacetate= 10: 1). Finally, compound (**7a**) (5.3 mg) was isolated in 18% yield. ¹H-NMR (400 MHz, (CD₃)₂SO) δ (ppm) 9.72 (s, 1H), 9.60 (s, 1H), 7.91 (d, *J* = 8.52 Hz, 2H), 7.73 (d, *J* = 8.52 Hz, 2H), 7.61 (dd, *J* = 7.88 Hz, *J* = 1.36 Hz, 1H), 7.05 (dt, *J* = 7.96 Hz, *J* = 1.60 Hz, 1H), 6.92 (dd, *J* = 8.08 Hz, *J* = 1.28 Hz, 1H), 6.83 (dt, *J* = 7.72 Hz, *J* = 1.32 Hz, 1H); ¹³C-NMR (100 MHz, (CD₃)₂SO) δ (ppm) 164.4,

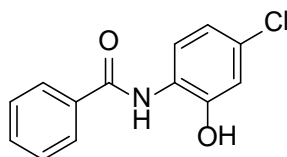
149.8, 133.6, 131.5, 129.8, 126.0, 125.6, 125.4, 124.7, 119.0, 116.0; LRMS (ESI) calcd for $C_{13}H_{10}BrNO_2[M+H]^+$: 291.99, found 291.95.



***N*-(2-hydroxyphenyl)benzamide (7b)**

1)Following the general procedure **I**, *N*-phenylbenzamide (20 mg, 0.1mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 50 °C in the sealed tube for 2.5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (Petroleum ether: Ethylacetate= 10: 1). Finally, compound (**7b**) (6.6 mg) was isolated in 31% yield.

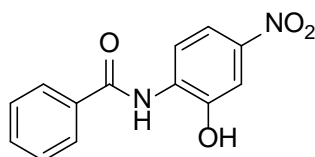
2)Following the general procedure **II**, *N*-phenylbenzamide (20 mg, 0.1mmol), $K_2S_2O_8$ (54 mg, 0.2 mmol) and $Pd(OAc)_2$ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 20 °C. in the sealed tube for 8 h. After completion of the reaction, the residue was purified by silica gel column chromatography (Petroleum ether: Ethylacetate= 10: 1). Finally, compound (**7b**) (6.8 mg) was isolated in 32% yield. 1H -NMR (400 MHz, $(CD_3)_2SO$) δ (ppm) 9.75 (s, 1H), 9.52 (s, 1H), 7.98 (d, $J = 7.20$ Hz, 2H), 7.70 (dd, $J = 8.00$ Hz, $J = 1.20$ Hz, 1H), 7.60 (t, $J = 7.20$ Hz, 1H), 7.53 (t, $J = 7.60$ Hz, 2H), 7.05 (dt, $J = 8.00$ Hz, $J = 1.20$ Hz, 1H), 6.94 (dd, $J = 8.00$ Hz, $J = 0.8$ Hz, 1H), 6.84 (dt, $J = 8.00$ Hz, $J = 1.20$ Hz, 1H); ^{13}C -NMR (100 MHz, $(CD_3)_2SO$) δ (ppm) 165.3, 149.3, 134.4, 131.7, 128.5, 127.5, 125.9, 125.7, 124.1, 119.0, 116.0; LRMS (ESI) calcd for $C_{13}H_{11}NO_2[M+H]^+$: 214.08, found 214.06.



***N*-(4-chloro-2-hydroxyphenyl)benzamide (7c)**

1)Following the general procedure **I**, *N*-(4-chlorophenyl)benzamide (24 mg, 0.1mmol), $K_2S_2O_8$ (81 mg, 0.3 mmol) and $[RuCl_2(p\text{-cymene})]_2$ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 50 °C in the sealed tube for 9 h. After completion of the reaction, the residue was purified by silica gel column chromatography (Petroleum ether: Ethylacetate= 10: 1). Finally, compound (**7c**) (12.6 mg) was isolated in 51% yield.

2)Following the general procedure **II**, *N*-(4-chlorophenyl)benzamide (24 mg, 0.1mmol), $K_2S_2O_8$ (54 mg, 0.2 mmol) and $Pd(OAc)_2$ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 50 °C. in the sealed tube for 5 h. After completion of the reaction, the residue was purified by silica gel column chromatography (Petroleum ether: Ethylacetate= 10: 1). Finally, compound (**7c**) (8.2 mg) was isolated in 33% yield. 1H -NMR (400 MHz, $(CD_3)_2SO$) δ (ppm) 10.29 (s, 1H), 9.50 (s, 1H), 7.96 (d, $J = 7.20$ Hz, 2H), 7.69 (d, $J = 8.80$ Hz, 1H), 7.60 (t, $J = 7.60$ Hz, 1H), 7.53 (t, $J = 7.60$ Hz, 2H), 6.95 (d, $J = 2.40$ Hz, 1H), 6.89 (dd, $J = 8.40$ Hz, $J = 2.40$ Hz, 1H); ^{13}C -NMR (100 MHz, $(CD_3)_2SO$) δ (ppm) 165.2, 150.6, 134.2, 131.7, 129.0, 128.5, 127.5, 125.5, 125.0, 118.7, 115.5; LRMS (ESI) calcd for $C_{13}H_{10}ClNO_2[M+H]^+$: 248.04, found 248.01.



***N*-(2-hydroxy-4-nitrophenyl)benzamide (7d)**

1) Following the general procedure **I**, *N*-(4-nitrophenyl)benzamide (25 mg, 0.1 mmol), K₂S₂O₈ (81 mg, 0.3 mmol) and [RuCl₂(*p*-cymene)]₂ (5 mol%, 0.005 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 60 °C in the sealed tube for 6 h. After completion of the reaction, the residue was purified by silica gel column chromatography (Petroleum ether: Ethylacetate= 10: 1). Finally, compound (**7d**) (12.1 mg) was isolated in 47% yield.

2) Following the general procedure **II**, *N*-(4-nitrophenyl)benzamide (25 mg, 0.1 mmol), K₂S₂O₈ (54 mg, 0.2 mmol) and Pd(OAc)₂ (10 mol%, 0.01 mmol) were used with TFA: TFAA= 0.9 ml: 0.1 ml as solvent. The reaction mixture was stirred at 50 °C. in the sealed tube for 4 h, then 60 °C for 2h. After completion of the reaction, the residue was purified by silica gel column chromatography (Petroleum ether: Ethylacetate= 10: 1). Finally, compound (**7d**) (10.8 mg) was isolated in 42% yield. ¹H-NMR (400 MHz, (CD₃)₂SO) δ (ppm) 9.59 (s, 1H), 8.23 (d, *J* = 9.20 Hz, 1H), 7.97 (d, *J* = 7.60 Hz, 2H), 7.79 (dd, *J* = 8.80 Hz, *J* = 2.40 Hz, 1H), 7.74 (d, *J* = 2.40 Hz, 1H), 7.64 (t, *J* = 7.20 Hz, 1H), 7.56 (t, *J* = 7.60 Hz, 2H); ¹³C-NMR (100 MHz, (CD₃)₂SO) δ (ppm) 165.4, 148.4, 143.4, 133.9, 133.0, 132.2, 128.7, 127.6, 121.7, 115.0, 109.5; LRMS (ESI) calcd for C₁₃H₁₀N₂O₄[M+H]⁺: 259.06, found 259.01.

Computational part:

Computational details

All the calculations were carried out with the Gaussian 09 package.¹ Geometry optimizations were performed with B3LYP². LANL2DZ+f (1.235 for Ru, 1.472 for Pd) basis set³ with effective core potential (ECP) was used for Pd and Ru, and the 6-31G (d) basis set⁴ was used for other atoms. Frequency was calculated at the same level of theory to obtain zero-point energy (ZPE) corrections and to verify the stationary points to be minima or saddle points. Single-point energies were conducted by using B3LYP/[SDD⁵ for Pd and Ru, 6-311++G(d,p)⁶ for others]. Solvent effects were evaluated with SMD solvation model (Solvent=Acetic Acid).⁷ The relative energies with ZPE corrections and free energies (at 298.15K) are in kcal/mol.

1. Potential energy surface (PES) of C-H activation

Potential energy surface (PES) and related structures of Pd and Ru Catalyzed C-H Activation are shown in **Figures S1** and **S2**, respectively. Free energies ΔG (electronic energies Δ(E+ZPE) in parentheses) are in kcal/mol. Since our previous KIE experiment revealed that the C-H activation step is involved in the rate-determining step⁸⁻⁹, we envisage that the relative energy between different transition states of C-H cleavage may determine the regioselectivity, the elementary steps after the C-H activation step had not been considered. Recent mechanistic studies on the carboxylate-assisted transition-metal catalyzed C-H activation supported that the concerted metalation-deprotonation (CMD) mechanism with an inner- or outer-sphere base was the most favorable mechanism (abbreviated as innersphere_CMD and outersphere_CMD respectively).¹¹ For Pd, the Δ(E+ZPE)[‡] of the outersphere_CMD mechanism is more favorable than the innersphere_CMD mechanism. It has been noticed, if the number of molecules changes during the reaction, the entropy contribution to the reaction Gibbs energy change is largely overestimated¹², Δ(E+ZPE)[‡] is preferred over ΔG[‡] to describe the change of energy. Therefore, the outersphere_CMD was chosen as the mechanism for C-H activation for Pd catalyst. However, for Ru, whether considering Δ(E+ZPE)[‡] or ΔG[‡], the innersphere_CMD mechanism has lower energy barrier than the outersphere_CMD mechanism. Therefore, the innersphere_CMD mechanism is more favorable for Ru catalyst.

The agostic interactions have been considered. **INT1-ag**, **INT2-ag**, **TS3-ag**, **TS4-ag**, **INT3-ag**, and **INT4-ag** are relevant structures (Figures S1 and S2). The energies of transition states of agostic interactions are about lower

than these of C-H activation. Therefore, the C-H activation step is still the rate-determining step which is also consistent with the KIE results and the regioselectivity could not be influenced by the agnostic interactions.

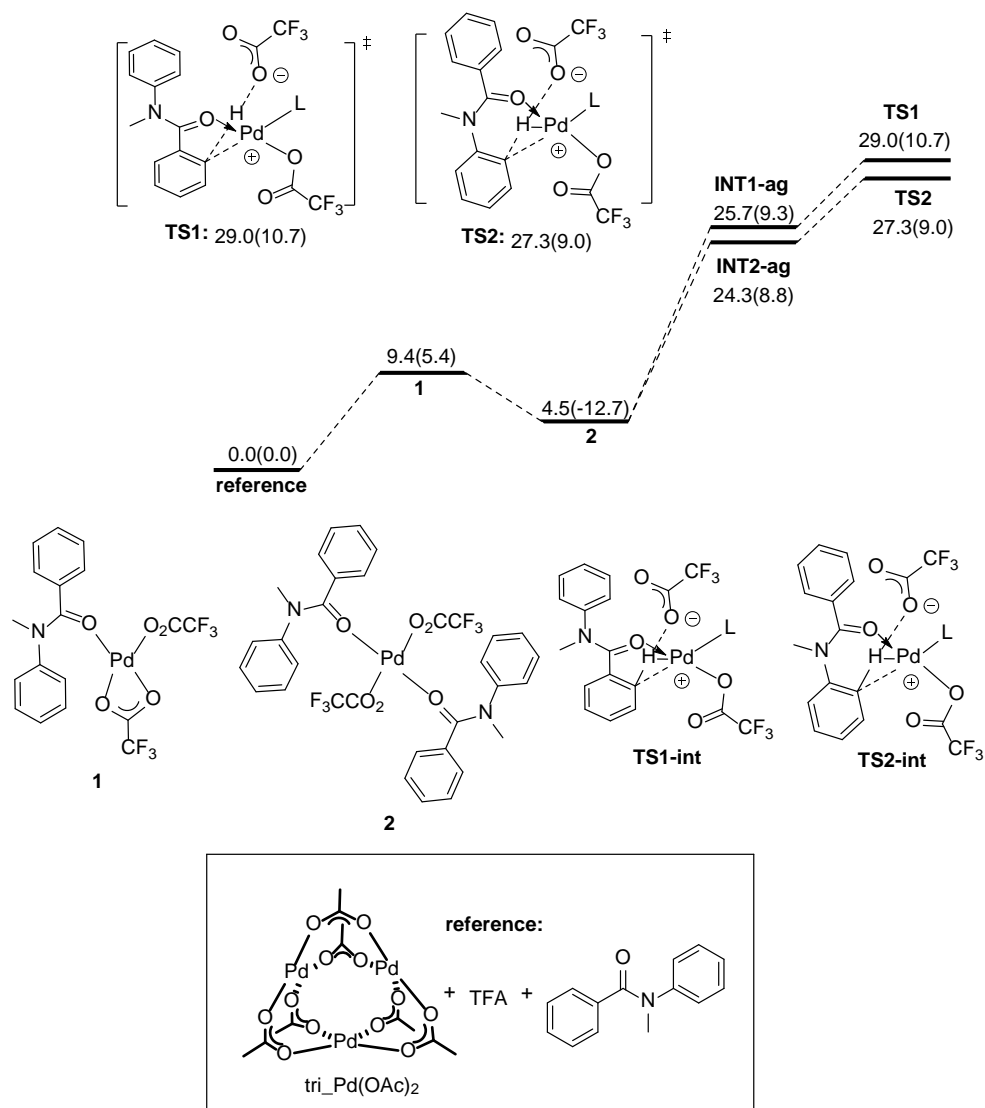


Figure S1. Potential energy surface and related structures for Pd catalyst (in kcal/mol).

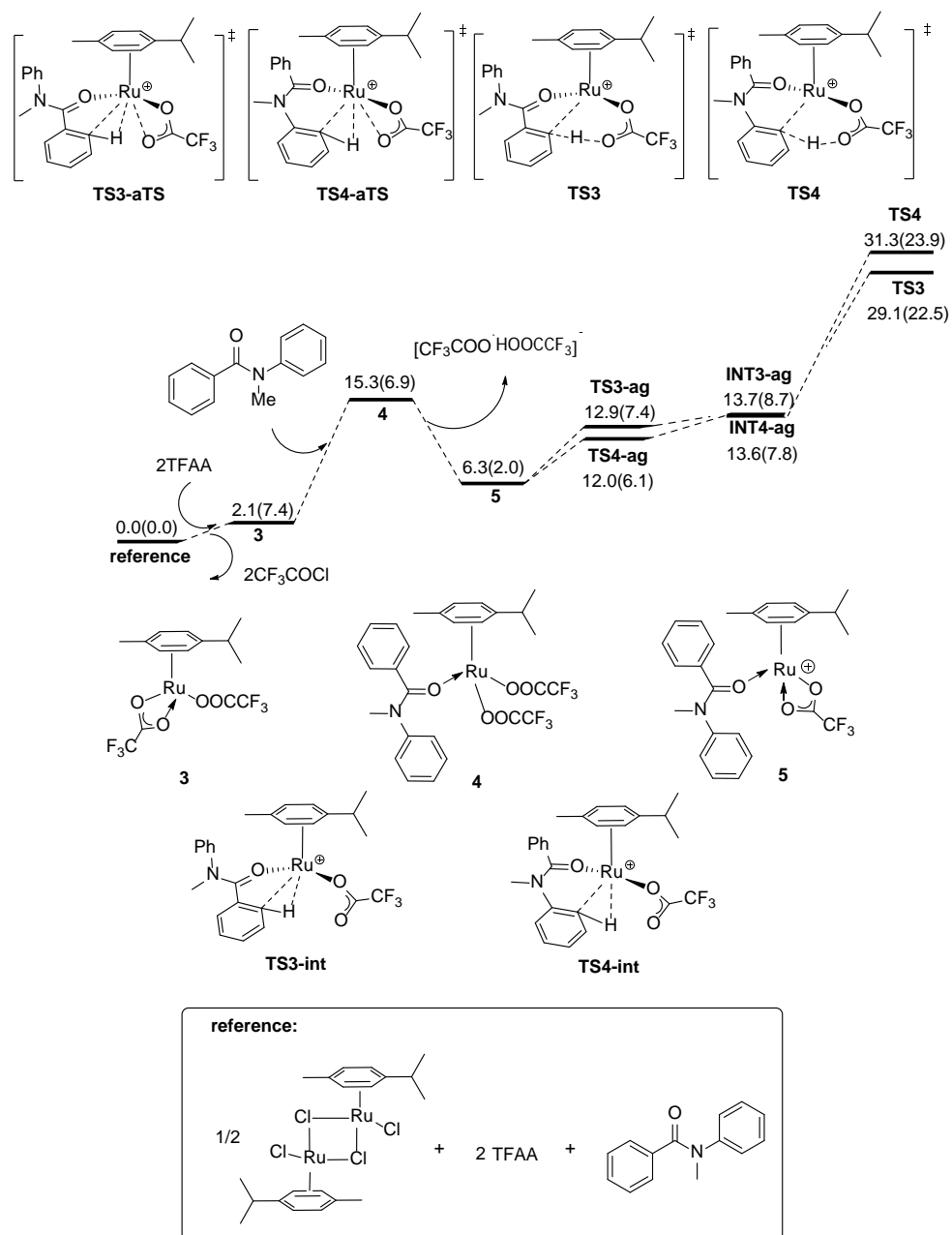


Figure S2. Potential energy surface and related structures for Ru catalyst (in kcal/mol).

2. Model calculations to examine the role of steric factor in Ru-catalyzed transition states

As shown in **Figure S3**, calculations were performed on models to verify if the steric factor is important. Firstly, the p-cymene cap was replaced by three carbon monoxide, which is much smaller. The steric repulsion between the cap and the activated benzene ring are therefore largely eliminated. In this case, the regioselectivity is reversed, i.e. TS4_3CO becomes preferred. Moreover, to a further extreme, the p-cymene cap was deleted to eliminate the steric factor completely. The computational results reveal that the regioselectivity is reversed (**TS3_no_cap** and **TS4_no_cap**). Therefore, the conclusion was drawn that steric repulsion plays an important role for the regioselectivity.

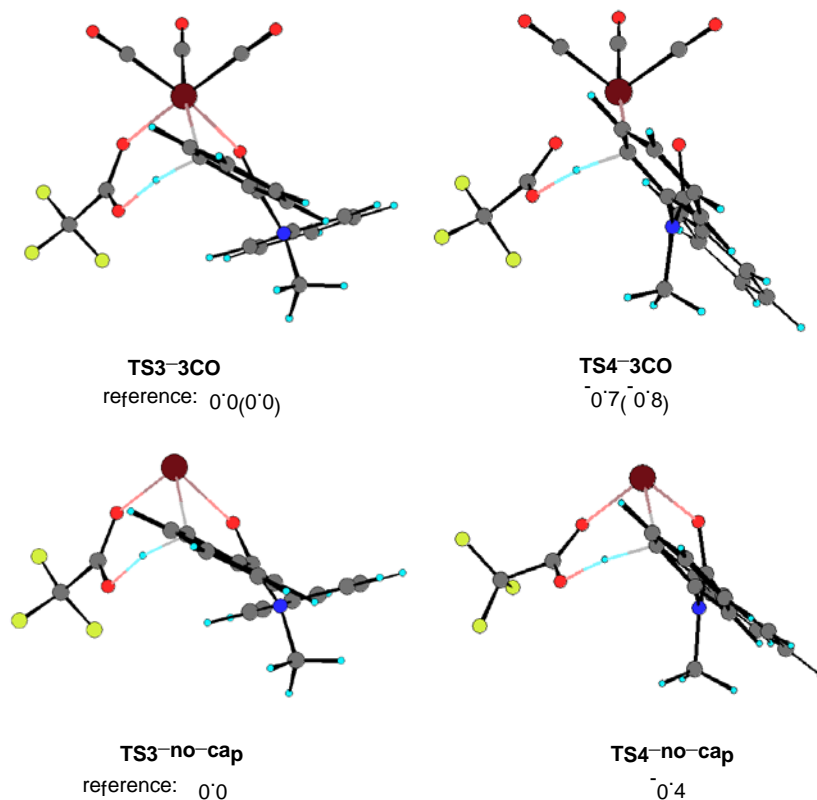


Figure S3. Relative energies (in kcal/mol) of the transition state of Ru-catalyzed C-H activation on model systems.

3. Energies of Optimized Molecular Structures

Activation free energies (activation electronic energies in parentheses) are in kcal/mol.

Geometry	E(M06)+ZPE	G	$\Delta(E+ZPE)$	ΔG
[RuCl ₂ (p-cymene)] ₂	-2809.77756	-2809.841026	0.0	0.0
TFA	-526.9291171	-526.9606541	--	--
TFAA	-977.387229	-977.428868	--	--
N-methyl-benzanilide	-671.2495917	-671.2911697	--	--
CF ₃ COCl	-911.2947495	-911.3268495	--	--
HCl	-460.8322102	-460.8501022	--	--
[CF ₃ COO·OOCCF ₃] [·]	-1053.443008	-1053.489274	-14.5	-3.8
CF ₃ COO [·]	-526.4907995	-526.5226265	--	--
TS0	-1357.231807	-1357.291296	--	--
1	-1851.88095	-1851.948495	5.4	9.4
2	-2523.159371	-2523.247436	-12.7	4.5
3	-1537.061965	-1537.121141	7.4	2.1
TS3-aTS	-1681.797701	-1681.866528	7.4	12.9
TS4-aTS	-1681.799642	-1681.867991	6.1	12.0
TS3-int	-1681.795608	-1681.865232	8.7	13.7
TS4-int	-1681.796952	-1681.865378	7.8	13.6
TS3	-1681.773632	-1681.840801	22.5	29.1
TS4	-1681.771305	-1681.837244	23.9	31.3
tri_Pd(OAc) ₂	-1754.988215	-1755.060059	0.0	0.0
4	-2208.312369	-2208.39126	6.9	15.3
5	-1681.806259	-1681.877102	2.1	6.3
TS1-int	-2523.124246	-2523.078864	9.3	25.7
TS2-int	-2523.12511	-2523.215926	8.8	24.3
TS1	-2523.12202	-2523.208406	10.7	29.0
TS2	-2523.124721	-2523.211112	9.0	27.3
TS1_inner	-1851.854365	-1851.921541	22.0	26.3
TS2_inner	-1851.860918	-1851.925594	17.9	23.8
TS3_benzene	-1524.574656	-1524.634275	--	--
TS3_p-dimethylbenzene_cf1	-1603.180839	-1603.244986	--	--
TS3_p-dimethylbenzene_cf2	-1603.182109	-1603.245493	--	--
TS3_p-dimethylbenzene_cf3	-1603.180715	-1603.243827	--	--
TS3_cf2	-1681.771963	-1681.8384	--	--
TS3_cf3	-1681.772531	-1681.839198	--	--
TS4_benzene	-1524.572608	-1524.632257	--	--
TS4_p-dimethylbenzene_cf1	-1603.177386	-1603.240831	--	--
TS4_p-dimethylbenzene_cf2	-1603.180211	-1603.243096	--	--
TS4_p-dimethylbenzene_cf3	-1603.180207	-1603.243091	--	--
TS4_cf2	-1681.769887	-1681.836695	--	--
TS4_cf3	-1681.768873	-1681.83495	--	--

TS3_outer	-2208.276118	-2208.354534	29.6	38.4
TS4_outer	-2208.277787	-2208.356248	28.6	37.3
TS5	-1642.496537	-1642.56381	24.6	29.9
TS6	-1642.497389	-1642.56506	24.1	29.1
TS5_no_H	-1642.049475	-1642.113308	52.7	48.2
TS6_no_H	-1642.036501	-1642.102636	44.6	41.5
TS3_3CO	-1632.480182	-1632.542028		
TS4_3CO	-1632.481311	-1632.543192		
TS3_no_cap (only E(B3LYP))	-1292.576263	--	--	--
TS4_no_cap (only E(B3LYP))	-1292.576852	--	--	--

4. Reference

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5. Cartesian Coordinates

[RuCl₂(*p*-cymene)]₂

C	3.24504600	1.27032300	0.02557800
C	3.37150300	0.42130500	-1.09342600
C	3.63933000	-0.97963800	-0.93638000
C	3.82019800	-1.56853000	0.33790300
C	3.65826400	-0.71291600	1.48262700
C	3.36721700	0.66059500	1.32729800
H	3.15967700	0.80157500	-2.08509200
H	3.65926000	-1.15063000	2.47501900
Ru	1.84969700	-0.50677900	0.25852000
H	3.63536000	-1.61516100	-1.81610500
H	3.15571800	1.25769600	2.20874000
Cl	0.28708900	-0.94317100	-1.64516500
Cl	-0.02165800	0.99444300	0.96207200
C	-2.48423600	-2.00889900	0.02773200
C	-3.03746700	-1.68353100	-1.25994700
C	-3.75556400	-0.46853200	-1.38802700
C	-3.91706600	0.41568900	-0.27257500
C	-3.36151300	0.10505800	0.99341400
C	-2.64092200	-1.13707200	1.11958500
H	-1.81635600	-2.85702200	0.13022800
H	-4.37160000	1.38369300	-0.44256900
Ru	-1.77756400	0.01964800	-0.57000500
H	-4.09676300	-0.14896300	-2.36657800
H	-2.09044100	-1.34696300	2.03052000
Cl	0.76957800	-2.30621500	1.50470700
Cl	-1.51927800	1.96707300	-1.97674700
C	4.07358500	-3.04003300	0.50939700
H	3.38141400	-3.46018400	1.24543700
H	3.93695300	-3.57594000	-0.43387600
H	5.10151600	-3.20825600	0.85527500
C	-2.80487200	-2.58573000	-2.44075000
H	-2.93423900	-2.04634100	-3.38302500
H	-1.79496800	-3.00416000	-2.41749800
H	-3.52163800	-3.41722400	-2.41853800
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H	2.24609800	2.98416200	0.74029300
C	2.26462300	3.17099300	-1.38961600
H	1.33420300	2.62069600	-1.56146800
H	2.01691500	4.23693900	-1.34542000
H	2.92887100	3.03126100	-2.25207900
C	4.24308200	3.54980500	0.16357000
H	4.02806800	4.62391100	0.16958600

H	4.71042800	3.29338900	1.12156300
H	4.97368500	3.35639500	-0.63116400
C	-3.46252200	1.03125800	2.19310100
H	-2.52468600	0.91460500	2.75011100
C	-4.61759400	0.56076300	3.10324400
H	-4.49230800	-0.48325100	3.41164600
H	-4.65842900	1.17796500	4.00765600
H	-5.58290800	0.64914600	2.59000700
C	-3.60681600	2.51521600	1.82776000
H	-3.53287600	3.12441500	2.73506300
H	-2.82194200	2.83341200	1.13438300
H	-4.58118800	2.73137200	1.37256500

TFA

C	-0.60094700	-0.00076000	-0.00019600
C	0.93423300	0.16007000	-0.00057500
O	1.49777700	1.22253700	-0.00032900
O	1.52071400	-1.04590600	-0.00027800
F	-1.18853800	1.19603200	-0.00239000
F	-0.99710400	-0.68234900	-1.08848100
F	-0.99584800	-0.67741500	1.09183400
H	2.48575300	-0.89531000	0.00081100

TFAA

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C	1.19488800	0.68985100	0.16595300
O	1.34035600	1.83536100	0.45434500
F	2.26479600	-0.85605000	-1.27267500
F	3.51543700	0.28737200	0.09770300
F	2.24785400	-1.31310600	0.85966100
O	0.00000000	0.01578900	0.00000700
C	-1.19488600	0.68985000	-0.16595400
O	-1.34035300	1.83535900	-0.45434600
C	-2.34188300	-0.32485000	0.04293600
F	-3.51543600	0.28737200	-0.09771700
F	-2.24785000	-1.31311300	-0.85965300
F	-2.26480400	-0.85603900	1.27267800

N-methyl-benzanilide

C	4.65882900	-0.29208100	-0.17756300
C	4.19638700	0.92197700	0.33765200
C	2.82913900	1.18825700	0.37781800
C	1.90615000	0.22981600	-0.06405200
C	2.37722400	-0.98205600	-0.58808900

C	3.74767600	-1.23830200	-0.65057300
H	5.72552400	-0.49552300	-0.21889000
H	4.90250700	1.66568100	0.69687200
H	1.67420900	-1.71676400	-0.96994300
H	4.10282400	-2.17479200	-1.07215900
C	0.44964400	0.62232600	-0.09460800
O	0.14398700	1.72513000	-0.53494800
N	-0.48703700	-0.29920300	0.35919400
C	-0.10605700	-1.45841900	1.17567200
H	-0.84615000	-1.58453500	1.97090300
H	-0.05573700	-2.39064800	0.59982900
H	0.86875300	-1.28666200	1.63054000
C	-1.89049600	-0.11885000	0.12725800
C	-2.67937300	-1.25497200	-0.11398400
C	-2.50743700	1.14175700	0.16641300
C	-4.05427100	-1.13634200	-0.31386800
H	-2.21895500	-2.23667400	-0.15921100
C	-3.88264100	1.24827100	-0.04206200
H	-1.91125700	2.02436300	0.34416100
C	-4.66481400	0.11741900	-0.28135800
H	-4.64431900	-2.02943800	-0.50203300
H	-4.34459100	2.23151300	-0.00885300
H	-5.73551100	0.21192900	-0.43954600
H	2.46029400	2.14213200	0.74163300

CF3COCl

C	0.86758300	-0.14622100	-0.00001600
C	-0.46969200	0.64129800	-0.00009200
O	-0.53755600	1.82574700	0.00005800
F	1.88649200	0.71220600	-0.00094900
F	0.94324500	-0.92016600	1.09017100
F	0.94273400	-0.92188800	-1.08888700
Cl	-1.88465500	-0.43575300	-0.00016700

HCl

Cl	0.00000000	0.00000000	0.07163900
H	0.00000000	0.00000000	-1.21785500

1

C	5.04388800	0.01575600	-2.60500100
C	4.43599000	1.18313600	-3.07304000
C	3.49369300	1.84556300	-2.28517100
C	3.17144800	1.33242100	-1.02777900
C	3.77764100	0.17131000	-0.54714300

C	4.71135300	-0.48936700	-1.34621200
H	5.77207100	-0.50149300	-3.22339100
H	4.68766200	1.57516900	-4.05431900
H	3.00327800	2.74546600	-2.64598200
H	3.50289000	-0.21570700	0.42711900
H	5.16949800	-1.40373700	-0.98125100
N	2.22583900	2.04001700	-0.18691900
C	0.96486300	1.59032900	-0.08013700
O	0.59692800	0.65086100	-0.84767600
Pd	-0.95858100	-0.59828100	-0.38866400
C	-3.36967000	-0.63003600	-0.72154300
O	-2.78438700	-1.61532200	-0.18055700
O	-2.70793600	0.38766400	-1.08450100
C	1.21440400	-1.72294100	1.15422200
O	0.32177800	-1.99143800	0.26537600
C	2.12343600	-2.94411600	1.46931000
C	-4.88240300	-0.68286400	-0.98066600
O	1.45620600	-0.67256500	1.73705100
F	-5.48024100	-1.54474300	-0.15225300
F	-5.10454200	-1.07739700	-2.24733000
F	-5.42603400	0.53135700	-0.81309200
F	2.24347400	-3.10246100	2.79769300
F	1.68489700	-4.09493400	0.94687800
F	3.36377400	-2.70906900	0.97099400
C	2.75101800	3.21968700	0.51033600
H	3.47604400	2.91213200	1.27129200
H	3.25725600	3.86408400	-0.21398500
H	1.94151100	3.77307000	0.98256500
C	0.00846600	2.23988800	0.86677400
C	-1.12100700	2.88197300	0.33864100
C	0.20074600	2.18048400	2.25486300
C	-2.04138900	3.48325200	1.19697500
H	-1.27978900	2.90281900	-0.73495800
C	-0.73213400	2.77293300	3.10500400
H	1.04819600	1.63578200	2.65559500
C	-1.84772100	3.43000000	2.57882900
H	-2.91230500	3.98426300	0.78475200
H	-0.59095200	2.71388400	4.18037200
H	-2.56992500	3.89225100	3.24607800

2

C	5.82766500	-1.09471500	-2.34942100
C	5.47014900	0.09792000	-2.98246300
C	4.75864600	1.07423300	-2.28395400

C	4.41209100	0.84965400	-0.95034600
C	4.76901800	-0.33665300	-0.30718500
C	5.47343000	-1.31066900	-1.01587100
H	6.37708900	-1.85575000	-2.89673100
H	5.73730900	0.26704000	-4.02183000
H	4.46229100	1.99919200	-2.77096600
H	4.47642900	-0.49739500	0.72415900
H	5.73689300	-2.24081900	-0.52080600
N	3.71416600	1.88095300	-0.21113500
C	2.38721600	1.76693900	-0.00194700
O	1.77554200	0.83413100	-0.59443800
C	1.95549900	-1.27020400	1.80454200
O	0.96470700	-1.46999000	1.01570600
C	2.55659300	-2.59935300	2.34367900
O	2.50552100	-0.23121800	2.15540100
F	2.79360400	-2.51608600	3.66305300
F	1.77345300	-3.67628000	2.13532500
F	3.74152000	-2.83698800	1.72866600
C	4.54200100	2.99385500	0.26426900
H	5.22600200	2.64799800	1.04700300
H	5.13443200	3.38012000	-0.57053600
H	3.91474500	3.79063000	0.65952100
C	1.68334000	2.77270300	0.85265600
C	0.73030100	3.61300100	0.26105500
C	1.94952400	2.86654400	2.22693000
C	0.05992900	4.55555900	1.04073900
H	0.49254900	3.50974800	-0.79028500
C	1.26565800	3.80458500	2.99912700
H	2.65346900	2.17982400	2.68316600
C	0.32659000	4.65394300	2.40739600
H	-0.68161600	5.19925100	0.57657000
H	1.46188600	3.86656500	4.06593600
H	-0.20285800	5.38417500	3.01364700
C	-5.82693300	1.09407600	2.35080900
C	-5.46919500	-0.09867300	2.98350600
C	-4.75786300	-1.07482100	2.28459200
C	-4.41169600	-0.84996300	0.95092900
C	-4.76884800	0.33646500	0.30811100
C	-5.47309000	1.31031200	1.01719900
H	-6.37622500	1.85498200	2.89843200
H	-5.73605100	-0.26801300	4.02291500
H	-4.46134500	-1.99987400	2.77132600
H	-4.47655000	0.49743600	-0.72328000
H	-5.73673000	2.24055300	0.52240000

N	-3.71395100	-1.88110100	0.21132400
C	-2.38707300	-1.76695100	0.00170900
O	-1.77528300	-0.83419000	0.59412900
Pd	0.00008500	-0.00002000	-0.00022600
C	-1.95581100	1.27033300	-1.80452100
O	-0.96452800	1.46989800	-1.01624800
C	-2.55695000	2.59960200	-2.34332600
O	-2.50623200	0.23147800	-2.15513800
F	-2.79407400	2.51659000	-3.66270100
F	-1.77380100	3.67650400	-2.13483900
F	-3.74181500	2.83711000	-1.72816100
C	-4.54189000	-2.99391000	-0.26410800
H	-5.22596200	-2.64795700	-1.04674100
H	-5.13424700	-3.38022000	0.57072600
H	-3.91471900	-3.79068500	-0.65949600
C	-1.68341800	-2.77254800	-0.85328700
C	-0.73020900	-3.61296400	-0.26211700
C	-1.95002300	-2.86615000	-2.22749100
C	-0.06011100	-4.55541200	-1.04217300
H	-0.49211500	-3.50988900	0.78916600
C	-1.26641400	-3.80407100	-3.00006300
H	-2.65410600	-2.17934800	-2.68339100
C	-0.32719100	-4.65355800	-2.40876700
H	0.68153700	-5.19923400	-0.57834500
H	-1.46297300	-3.86586000	-4.06682200
H	0.20204600	-5.38370700	-3.01530100

3

C	-2.18337500	-1.29161100	1.28487700
C	-1.16444200	-2.29632300	1.30431100
C	-0.66738400	-2.84363100	0.09370000
C	-1.18833600	-2.33095300	-1.13150800
C	-2.20985800	-1.33710500	-1.12952100
C	-2.77599200	-0.82816800	0.07730500
H	-2.47222400	-0.82743100	2.22345400
H	-0.71449600	-2.58330600	2.24834700
H	-0.75271800	-2.64670700	-2.07320000
H	-2.50932600	-0.90819300	-2.07941300
C	-3.89113400	0.20464400	0.10792400
H	-3.73979500	0.79761600	1.01977100
C	-5.25329600	-0.51093800	0.23088400
H	-5.29274500	-1.15863600	1.11378500
H	-6.06099800	0.22463200	0.31302800
H	-5.45067400	-1.13077500	-0.65214600

C	-3.87787700	1.17200800	-1.08585900
H	-4.62014900	1.96116700	-0.92649200
H	-2.89806300	1.64166300	-1.21417100
H	-4.14402800	0.66616900	-2.02211300
C	0.50367800	-3.78706400	0.08298000
H	1.40520600	-3.24415400	-0.22542700
H	0.68169500	-4.20945300	1.07538400
H	0.33149700	-4.60745300	-0.62163300
Ru	-0.53100600	-0.57323100	0.04807100
O	1.50752600	-0.85745500	-0.08696800
C	2.49107600	-0.01498900	-0.13338400
O	2.49591300	1.20395800	-0.15405100
C	3.84303100	-0.78134700	-0.11941100
F	4.09575800	-1.24549900	1.12511900
F	4.86153200	0.00354700	-0.48519300
F	3.82006200	-1.84860600	-0.95066200
O	-0.12376800	1.21657500	1.18971000
C	-0.00897800	1.86120400	0.10756200
O	-0.31356800	1.30586300	-0.98983200
C	0.37075900	3.34545000	0.13300500
F	-0.77496700	4.06152200	0.26670200
F	0.96281100	3.72137100	-1.00134300
F	1.16202900	3.63305000	1.16733800

TS3-aTS

C	-1.08808500	-3.45797200	-2.82643300
C	-1.32095700	-2.10074900	-2.59684000
C	-0.38388500	-1.33509700	-1.89335800
C	0.80506700	-1.93222600	-1.43255600
C	1.03532900	-3.29335400	-1.66518700
C	0.08777100	-4.05131600	-2.35841000
H	-1.81264800	-4.05027800	-3.37706300
H	-2.21556900	-1.62111800	-2.98224900
H	-0.54677100	-0.25636800	-1.83272800
H	1.93933500	-3.76654600	-1.29278600
H	0.27082400	-5.10736100	-2.53318100
C	1.70215900	-1.12548500	-0.54695100
O	1.19427200	-0.61655000	0.49788200
N	3.00054900	-0.95097500	-0.81151300
C	3.66937200	-1.41620600	-2.03852600
H	4.20823500	-0.57220700	-2.47605500
H	4.38748000	-2.20816700	-1.80564400
H	2.93814800	-1.78670700	-2.75514800
C	3.81911300	-0.16595100	0.09674600

C	4.82728900	-0.80562800	0.81930700
C	3.62440900	1.21417300	0.19063800
C	5.65572100	-0.05058400	1.65151400
H	4.96201300	-1.88045100	0.73581300
C	4.45686400	1.95741500	1.02795100
H	2.83082800	1.69797200	-0.36974800
C	5.47152000	1.32950500	1.75507900
H	6.44298400	-0.54192000	2.21526800
H	4.31299500	3.03075000	1.10673600
H	6.11914700	1.91582500	2.40006500
C	-2.31118400	0.63863600	2.06849100
C	-1.24273100	-0.00944600	2.75845300
C	-0.99854500	-1.41733700	2.59481700
C	-1.78042200	-2.10918700	1.64115100
C	-2.76431400	-1.41445500	0.88022100
C	-3.11279300	-0.04878300	1.12105400
H	-2.42936900	1.71194100	2.18276600
H	-0.59085000	0.57457800	3.40040500
H	-1.55418200	-3.14312300	1.40534300
H	-3.24586000	-1.94215700	0.06480200
C	-4.24984900	0.66490200	0.40910600
H	-3.95604900	1.71828900	0.32363700
C	-5.50805800	0.58928500	1.30449400
H	-5.32735900	1.00709600	2.30096200
H	-6.32256700	1.15686700	0.84338800
H	-5.84560900	-0.44678500	1.42536000
C	-4.53910600	0.14755600	-1.00615400
H	-5.32813200	0.75741000	-1.45664000
H	-3.65295600	0.22894200	-1.64114400
H	-4.90107800	-0.88801300	-1.00093200
C	0.12600600	-2.08076800	3.33593600
H	1.01426200	-1.44246300	3.35723800
H	-0.18202300	-2.26392400	4.37319400
H	0.39353600	-3.03980200	2.88585600
Ru	-0.89529100	-0.27661100	0.65734000
O	-0.25361700	1.58200000	0.02942700
C	-0.77379600	2.13585200	-1.01723800
O	-1.62126400	1.67119500	-1.77066500
C	-0.14915500	3.52884200	-1.28451500
F	-0.29602500	4.32975800	-0.21461300
F	-0.70524900	4.11853700	-2.34156200
F	1.17667700	3.38976500	-1.52446500

TS4-aTS

C	-0.69797200	4.03119300	2.17967600
C	0.43186500	4.41007500	1.44425000
C	1.37245600	3.45414400	1.05832700
C	1.17567700	2.11396800	1.40710200
C	0.04654700	1.72133500	2.13617300
C	-0.88984600	2.69201000	2.52019100
H	-1.41324000	4.78344400	2.49958500
H	0.59045400	5.45355200	1.18789800
H	2.25994600	3.74227600	0.50252600
H	-0.08631700	0.68541400	2.43427900
H	-1.75339800	2.39241900	3.10705700
N	2.20336700	1.14885500	1.07877100
C	2.19962400	0.54856300	-0.12805600
O	1.21029700	0.67158900	-0.91484100
C	3.18835900	0.88814000	2.14493500
H	3.78731800	0.01507600	1.89328700
H	3.84095400	1.75539100	2.28597300
H	2.64846400	0.69976900	3.07644700
C	3.36346500	-0.24071500	-0.60205100
C	3.12224200	-1.50868200	-1.15720400
C	4.66706100	0.28199400	-0.58052800
C	4.18656000	-2.25478800	-1.65837800
H	2.11311600	-1.90747400	-1.15786800
C	5.72063700	-0.46006100	-1.11031400
H	4.85316100	1.27386200	-0.17810800
C	5.48203300	-1.73035600	-1.64225200
H	4.00490900	-3.24460500	-2.06601100
H	6.72516400	-0.04812600	-1.10919800
H	6.30666400	-2.31072500	-2.04556700
C	-2.14973200	-0.33042700	-2.09395800
C	-1.39113100	0.76650800	-2.59643100
C	-1.46731500	2.06898800	-1.99303200
C	-2.22661200	2.17162300	-0.81222900
C	-2.96019900	1.05273500	-0.28874100
C	-3.00147000	-0.19797600	-0.94790800
H	-2.01134000	-1.31055100	-2.54002900
H	-0.70127500	0.59932000	-3.41792400
H	-2.18745300	3.08722000	-0.23198100
H	-3.45527500	1.16288400	0.66857200
C	-3.80642800	-1.39300800	-0.46495600
H	-3.14245800	-2.26657800	-0.52033600
C	-4.97550700	-1.62527800	-1.45076200
H	-4.62719500	-1.76821300	-2.47956500
H	-5.52971600	-2.52224600	-1.15740400

H	-5.67216000	-0.77919700	-1.44078600
C	-4.31628500	-1.27091000	0.97684200
H	-4.82806900	-2.19646200	1.25725400
H	-3.49719800	-1.11540900	1.68499100
H	-5.04467500	-0.45740700	1.08095600
C	-0.65598800	3.21323600	-2.53023600
H	0.30892900	2.86670300	-2.91172600
H	-1.19435900	3.68970200	-3.35918000
H	-0.47711800	3.96825200	-1.76065300
Ru	-0.84908700	0.41675400	-0.55074200
O	-0.19027100	-1.51148800	-0.09900100
C	-0.50681800	-1.90755500	1.08661900
O	-1.02890400	-1.23058900	1.96985900
C	-0.22146600	-3.41195500	1.30436000
F	-1.13507900	-4.12881100	0.61376200
F	-0.30505900	-3.74486100	2.59251100
F	1.00135100	-3.74414600	0.85172800

TS3-int

C	1.15672600	-3.69241400	2.46954500
C	1.23718700	-2.30729400	2.60368900
C	0.30928600	-1.47583800	1.95579200
C	-0.71617800	-2.05366400	1.17551600
C	-0.79746400	-3.44716800	1.04820200
C	0.13561800	-4.25906400	1.69617900
H	1.86684200	-4.33382800	2.98291900
H	1.99734800	-1.86205400	3.23926700
H	0.25538600	-0.41270800	2.18298300
H	-1.58142300	-3.89443200	0.44363000
H	0.06204200	-5.33882000	1.60347100
C	-1.59033300	-1.15579300	0.34710700
O	-1.00898700	-0.47490800	-0.55327000
N	-2.91284800	-1.11678700	0.49035000
C	-3.63891500	-1.74762100	1.60416600
H	-4.13705600	-0.96548300	2.18375000
H	-4.39455800	-2.43405700	1.21229100
H	-2.95165600	-2.29005000	2.25195900
C	-3.70564900	-0.26383700	-0.37995300
C	-4.48348700	-0.85624700	-1.37558600
C	-3.71609000	1.11686200	-0.17394600
C	-5.28563400	-0.04913400	-2.18411900
H	-4.46211000	-1.93352300	-1.51650400
C	-4.51889000	1.91340800	-0.99153000
H	-3.09914800	1.55611500	0.60253000

C	-5.30303000	1.33410500	-1.99224400
H	-5.89551400	-0.50193700	-2.96007400
H	-4.52937700	2.98888500	-0.84245600
H	-5.92882400	1.96001200	-2.62148600
C	2.15600400	0.48184300	-2.05372700
C	1.44361700	-0.66938500	-2.48883700
C	1.67168300	-1.95818700	-1.90732000
C	2.56332000	-2.00254900	-0.81315000
C	3.29303200	-0.84543800	-0.37461400
C	3.14173100	0.40642000	-1.00851300
H	1.90136000	1.45003300	-2.47262100
H	0.65688300	-0.55137900	-3.22803800
H	2.65768400	-2.92307500	-0.24611300
H	3.92253200	-0.93106700	0.50291800
C	3.84785300	1.67393500	-0.56820100
H	3.09225000	2.46908600	-0.59939900
C	4.95314700	2.01089300	-1.59581800
H	4.55615200	2.09901400	-2.61305300
H	5.41836000	2.96640600	-1.33439300
H	5.73522500	1.24309700	-1.60029800
C	4.40874900	1.62092400	0.85825500
H	4.82225300	2.59913100	1.12093300
H	3.62852600	1.38493000	1.58968400
H	5.22153900	0.89117000	0.95646900
C	0.92430600	-3.17146900	-2.38656900
H	-0.08800900	-2.91228800	-2.71081600
H	1.44646100	-3.61176800	-3.24522400
H	0.85985400	-3.93403900	-1.60614100
Ru	1.10944400	-0.36551800	-0.36364100
O	0.76470900	1.52290300	0.39088000
C	-0.18536800	1.93250800	1.16571000
O	-0.95008500	1.27606800	1.86336300
C	-0.35358600	3.47580600	1.15500600
F	0.66637900	4.10864500	0.55482400
F	-0.46735600	3.94338300	2.40361700
F	-1.48675100	3.77695200	0.48306300

TS4-int

C	1.15050800	-3.64448600	2.26721300
C	-0.01960300	-4.20952500	1.74017800
C	-1.07242200	-3.39659000	1.32055200
C	-0.95606500	-2.00580200	1.42738200
C	0.21851000	-1.42239500	1.93497100
C	1.26768800	-2.26102600	2.36083100

H	1.95157500	-4.28753000	2.61962100
H	-0.11697900	-5.28914700	1.67111300
H	-1.98660100	-3.83197800	0.92837900
H	0.27879600	-0.35729000	2.15256500
H	2.15422900	-1.80699800	2.79362600
N	-2.10351900	-1.18545200	1.11767400
C	-2.20903400	-0.61278800	-0.09909200
O	-1.25674800	-0.66899400	-0.93253400
C	-3.05620100	-0.99165100	2.22703800
H	-3.76337100	-0.20527700	1.97068400
H	-3.59856000	-1.91897700	2.43584100
H	-2.49901400	-0.69806800	3.12070200
C	-3.45023900	0.08151300	-0.52108800
C	-3.32945700	1.37685700	-1.05063500
C	-4.70514000	-0.54605900	-0.46736300
C	-4.46686800	2.04492700	-1.49893400
H	-2.35640400	1.85685500	-1.06930700
C	-5.83252400	0.12030000	-0.94356800
H	-4.79609200	-1.55733100	-0.08045500
C	-5.71452000	1.41660400	-1.45286000
H	-4.37965200	3.05488500	-1.88774300
H	-6.80067000	-0.37043400	-0.91811000
H	-6.59659700	1.93689900	-1.81439500
C	1.96324000	0.36865300	-2.07899000
C	1.25431600	-0.74732100	-2.59464600
C	1.42812100	-2.06451500	-2.05059900
C	2.26803900	-2.17175000	-0.92363800
C	2.99449800	-1.04502000	-0.40706800
C	2.90140100	0.23283400	-0.99695300
H	1.74659800	1.35712500	-2.47146600
H	0.50507000	-0.58557200	-3.36354700
H	2.32514300	-3.11712300	-0.39539000
H	3.58900900	-1.17564000	0.48851000
C	3.68027400	1.44751800	-0.52458800
H	2.97811600	2.29153400	-0.51205300
C	4.77236500	1.76034800	-1.57564900
H	4.35256500	1.91655100	-2.57540400
H	5.30406300	2.67307300	-1.28942300
H	5.50421400	0.94671900	-1.63532100
C	4.28711900	1.30608700	0.87696000
H	4.76933500	2.24742300	1.15715800
H	3.52122300	1.09120300	1.62758100
H	5.06022100	0.52843800	0.90743200
C	0.66117000	-3.23522200	-2.59884300

H	-0.34118400	-2.93609700	-2.91904100
H	1.18431400	-3.64468700	-3.47207000
H	0.56820000	-4.03273400	-1.85684500
Ru	0.80238700	-0.53380600	-0.48616600
O	0.10868100	1.32705000	0.14047400
C	0.53339200	1.97556400	1.17662900
O	1.17472500	1.55852200	2.13240000
C	0.17664700	3.48079000	1.07376500
F	0.98969700	4.05110200	0.15185300
F	0.34792200	4.11149800	2.23428200
F	-1.09567300	3.66185400	0.67010700

TS3

C	0.90287700	-3.08491900	3.11220600
C	1.32236600	-1.96024100	2.39751600
C	0.45303200	-1.28038700	1.52436800
C	-0.89283800	-1.74188600	1.44702900
C	-1.30841200	-2.88213100	2.13962600
C	-0.40288300	-3.55769000	2.96440800
H	1.59214400	-3.59668800	3.77781200
H	2.33746300	-1.59465900	2.53169200
H	0.50633200	0.05713100	1.75616700
H	-2.31500100	-3.27096300	2.02758000
H	-0.72408100	-4.44735100	3.49774500
C	-1.72060600	-0.97560400	0.47761400
O	-1.10567700	-0.46753600	-0.51523300
N	-3.04037800	-0.76916200	0.59994800
C	-3.84190500	-1.10222100	1.78944800
H	-4.53715900	-0.27853200	1.96364400
H	-4.42145000	-2.01852800	1.63417400
H	-3.20245300	-1.21407800	2.66449500
C	-3.74259500	-0.05050500	-0.44940800
C	-4.54077100	-0.76724600	-1.34161100
C	-3.66102200	1.34228400	-0.51369700
C	-5.26716400	-0.07865000	-2.31537000
H	-4.59385800	-1.85026700	-1.27379900
C	-4.38812300	2.02069500	-1.49213000
H	-3.03360800	1.88722400	0.18501400
C	-5.19143200	1.31333300	-2.39040000
H	-5.89227100	-0.63072900	-3.01075400
H	-4.32887700	3.10341700	-1.54920900
H	-5.75925600	1.84735900	-3.14641800
C	2.16402300	0.13228100	-2.32433500
C	1.26688400	-0.89208200	-2.66019700

C	1.26802200	-2.14735900	-1.95081000
C	2.20249600	-2.30089000	-0.90434200
C	3.10349600	-1.24421500	-0.54646500
C	3.09900700	-0.01209100	-1.23794400
H	2.07690100	1.09501900	-2.81800300
H	0.50997700	-0.71150300	-3.41703700
H	2.19309300	-3.20910600	-0.31127600
H	3.75735200	-1.38142700	0.30611800
C	4.01360600	1.15035100	-0.89057300
H	3.42132300	2.06282800	-1.03766100
C	5.19196400	1.18217900	-1.89001800
H	4.84669500	1.23773500	-2.92808000
H	5.81826500	2.05895000	-1.69708800
H	5.81825300	0.28857600	-1.78723500
C	4.51834000	1.14580000	0.55881000
H	5.07666500	2.06642200	0.75374500
H	3.69400900	1.09666100	1.27922200
H	5.20149000	0.31049700	0.75311000
C	0.29090400	-3.23141300	-2.31405000
H	-0.67981800	-2.81003500	-2.59159900
H	0.66781800	-3.79825200	-3.17466700
H	0.14547700	-3.93090900	-1.48638900
Ru	1.00761800	-0.46361700	-0.46878400
O	0.68745700	1.59931600	-0.03097500
C	0.39683400	1.98198600	1.12832100
O	0.30824900	1.25504800	2.15725300
C	0.05050600	3.47650300	1.31103100
F	0.54793800	4.21428300	0.31636800
F	0.51692400	3.93517700	2.47348400
F	-1.29462400	3.59549300	1.30604000
TS4			
C	0.67270000	-3.30269500	2.93329100
C	-0.70006800	-3.51068400	3.09250400
C	-1.61095100	-2.65890400	2.47070800
C	-1.15644400	-1.60741400	1.66663200
C	0.22712800	-1.39626400	1.43205500
C	1.11262400	-2.26915600	2.11458300
H	1.38668600	-3.93820100	3.44864000
H	-1.06453800	-4.32353000	3.71363000
H	-2.67505600	-2.81753100	2.61318000
H	0.54511300	-0.09586100	1.76125400
H	2.18151000	-2.10062300	2.02184400
N	-2.15993300	-0.70441700	1.16205300

C	-2.21737700	-0.35901500	-0.14591300
O	-1.26884800	-0.58767900	-0.94777400
C	-3.11089100	-0.17119800	2.16217700
H	-3.56581300	0.74162000	1.78151000
H	-3.90177100	-0.88679000	2.40205800
H	-2.55084100	0.05820800	3.07113400
C	-3.42902800	0.28789700	-0.71469400
C	-3.25012400	1.38436500	-1.57399600
C	-4.71882400	-0.21957300	-0.48899000
C	-4.35506100	1.98704700	-2.17060600
H	-2.24886500	1.76337000	-1.75225000
C	-5.81708600	0.37211200	-1.10961600
H	-4.86162400	-1.08999700	0.14443500
C	-5.63728700	1.48021900	-1.94201300
H	-4.21665200	2.84754000	-2.81810700
H	-6.81140300	-0.03216600	-0.94631600
H	-6.49644500	1.94544800	-2.41618300
C	2.00766700	0.06207900	-2.35894100
C	1.16958200	-0.98323300	-2.76647800
C	1.17532000	-2.25453900	-2.08888600
C	2.06684900	-2.40827500	-1.00542200
C	2.92342200	-1.33904100	-0.58465600
C	2.89845900	-0.08553900	-1.23565700
H	1.91533000	1.03447600	-2.83206600
H	0.43839900	-0.80710200	-3.54921100
H	2.06008500	-3.33436700	-0.44093700
H	3.56072500	-1.48145100	0.27902100
C	3.75635100	1.09705200	-0.81569300
H	3.11751600	1.98651700	-0.89163300
C	4.91950300	1.26012000	-1.82009900
H	4.56104500	1.37133700	-2.84911000
H	5.50260300	2.15213400	-1.57003000
H	5.59199300	0.39529100	-1.78636800
C	4.28060100	1.02120900	0.62499000
H	4.78596300	1.95797800	0.87791900
H	3.47428500	0.87397900	1.35169400
H	5.01366200	0.21581000	0.75177700
C	0.24840400	-3.35503600	-2.52639200
H	-0.74601900	-2.96206900	-2.75852100
H	0.64083000	-3.83212300	-3.43330600
H	0.14882900	-4.12429800	-1.75618300
Ru	0.79030600	-0.62715800	-0.56567900
O	0.43575400	1.42894900	-0.01730700
C	0.56432800	1.81653500	1.16905000

O	0.66465600	1.07703500	2.19027300
C	0.67803200	3.34353900	1.37698900
F	1.91269300	3.72356600	0.98983800
F	0.50121100	3.68351000	2.65185600
F	-0.22267700	3.98316600	0.62125500

tri_Pd(OAc)₂

Pd	1.61508100	0.92607500	-0.01063700
C	-0.06180400	2.60426100	-1.87704500
O	1.04306300	2.41870300	-1.28785500
O	-1.17047300	2.03750200	-1.63766000
C	-2.27679100	-1.26108000	1.89219700
O	-1.54781200	-2.11771700	1.31084200
O	-2.35771900	-0.01908700	1.65045800
C	-3.18399200	-1.78937100	2.98645000
H	-3.45042500	-0.98878100	3.67891400
H	-4.10289000	-2.16823500	2.52377000
H	-2.70064700	-2.61478800	3.51312400
C	-0.06696100	3.64838100	-2.97668900
H	0.89297200	3.65373300	-3.49714400
H	-0.88619600	3.46227800	-3.67360100
H	-0.21637400	4.63426600	-2.52102100
Pd	-0.00137800	-1.86134600	-0.00019000
C	-2.26830100	-1.34837800	-1.84767700
O	-2.65299300	-0.30004400	-1.24903300
O	-1.22867100	-2.03454400	-1.61581500
C	0.06542900	2.60373200	1.87744000
O	1.17302800	2.03486200	1.63814400
O	-1.03965000	2.42052700	1.28788700
C	0.07253800	3.64762800	2.97728000
H	-0.88894700	3.65807400	3.49473400
H	0.88862700	3.45702500	3.67668800
H	0.22896100	4.63274300	2.52228300
C	-3.15645100	-1.82484800	-2.98071100
H	-3.11492800	-1.09396100	-3.79533600
H	-2.83124200	-2.80057800	-3.34375000
H	-4.19318200	-1.87436200	-2.63540100
Pd	-1.61369500	0.92869800	0.01071500
C	2.26616900	-1.35186200	1.84764700
O	2.65264100	-0.30415100	1.24904200
O	1.22555600	-2.03644500	1.61553300
C	3.15312800	-1.82951600	2.98111100
H	3.10978700	-1.09997000	3.79686100
H	2.82802700	-2.80599900	3.34223200

H	4.19039200	-1.87769400	2.63727400
C	2.27526300	-1.26390900	-1.89247000
O	2.35840500	-0.02211100	-1.65036800
O	1.54464200	-2.11937000	-1.31148500
C	3.18165900	-1.79352200	-2.98674800
H	4.09934900	-2.17515200	-2.52394700
H	2.69647400	-2.61728200	-3.51433700
H	3.45043300	-0.99303600	-3.67842000

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C	-2.42474000	0.86239700	2.09521300
C	-1.27013000	1.50374100	2.64282100
C	-0.15583200	0.73506100	3.04262600
C	-0.23534300	-0.69704100	2.92878600
C	-1.39040000	-1.31729800	2.41512800
C	-2.53321700	-0.55191600	1.99843800
H	-3.21245000	1.47524200	1.67302800
H	-1.20307700	2.58595900	2.62993600
H	0.64508000	-1.29522700	3.13741300
H	-1.37244800	-2.38568500	2.23484500
C	-3.81795600	-1.18653200	1.49241600
H	-4.22843600	-0.50367700	0.74206800
C	-4.82373200	-1.27232700	2.66182100
H	-5.01975000	-0.28919100	3.10467200
H	-5.77664300	-1.67900800	2.30533300
H	-4.45191300	-1.93353900	3.45431600
C	-3.62648900	-2.55672800	0.82707900
H	-4.57867400	-2.88578300	0.39708000
H	-2.88317700	-2.51515700	0.02823400
H	-3.32219800	-3.32186000	1.55309800
C	1.11003500	1.38462300	3.53024100
H	1.21606600	2.39817100	3.13416600
H	1.09749200	1.44240500	4.62653300
H	1.98611900	0.80175600	3.23328100
Ru	-0.70872800	0.17680800	0.93247500
O	-0.78147200	-1.30888700	-0.51903500
C	-0.22003800	-1.31680000	-1.67830000
O	0.48832900	-0.49488900	-2.24224900
C	-0.48190400	-2.67342100	-2.39649500
F	0.35860500	-3.62084600	-1.89759600
F	-0.25628100	-2.59002700	-3.71338700
F	-1.73982300	-3.12550100	-2.22066500
O	-1.51708900	2.80490600	-2.35237100
C	-1.75836100	1.95765200	-1.50552800

O	-0.98703800	1.61814600	-0.53089700
C	-3.16135000	1.28547400	-1.57221000
F	-3.94327400	1.72329500	-0.53644000
F	-3.11042600	-0.06228800	-1.47025200
F	-3.80599100	1.58188800	-2.70217300
C	2.14101300	5.00722500	-0.81215600
C	2.92689300	4.53929200	0.24566800
C	3.03253100	3.16826000	0.47768100
C	2.34206000	2.26329100	-0.34484700
C	1.55738800	2.73164900	-1.40269000
C	1.46119900	4.10526900	-1.63188900
H	2.05636000	6.07590500	-0.99159500
H	3.45697900	5.23890400	0.88663700
H	1.01414400	2.02993900	-2.02149700
H	0.82274900	4.45597300	-2.43576700
C	2.41145800	0.79727900	-0.04358900
O	1.46313600	0.16094600	0.46419800
N	3.58745900	0.15225000	-0.26162000
C	4.72654300	0.72542500	-0.98695500
H	5.60659100	0.78564300	-0.33694600
H	4.96648600	0.08334200	-1.84055800
H	4.47874900	1.72173500	-1.34775400
C	3.71438400	-1.24216000	0.09402100
C	3.09674700	-2.22269900	-0.68484900
C	4.50102400	-1.59672400	1.19253000
C	3.26016200	-3.56721100	-0.35058700
H	2.48421700	-1.92611300	-1.52871600
C	4.66898800	-2.94494100	1.51548600
H	4.97582600	-0.82125800	1.78813200
C	4.04764800	-3.93027400	0.74500900
H	2.76228600	-4.32536300	-0.94688300
H	5.28296000	-3.22275300	2.36793700
H	4.17621000	-4.97899900	0.99871300
H	3.64856000	2.79947300	1.29494900

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C	2.80915700	-0.67504500	-1.72521100
C	1.80969400	-1.51151100	-2.28496000
C	1.18732000	-2.53119900	-1.49828100
C	1.57437300	-2.64835900	-0.14080400
C	2.58411700	-1.79601800	0.40996000
C	3.25385700	-0.81604000	-0.37088600
H	3.19228400	0.15045400	-2.31816800
H	1.46318200	-1.32745000	-3.29604900

H	1.04091700	-3.33173700	0.51104900
H	2.77837700	-1.85050400	1.47514300
C	4.34443700	0.09413000	0.16887600
H	4.20868500	1.06752000	-0.32092400
C	5.71918300	-0.46556800	-0.26175000
H	5.79209600	-0.57955000	-1.34883900
H	6.51400000	0.21514400	0.05939300
H	5.90615600	-1.44363800	0.19645600
C	4.29015100	0.31687500	1.68734100
H	5.04960900	1.05130400	1.97217300
H	3.31839800	0.69742600	2.01837200
H	4.51048900	-0.60207700	2.24337300
C	0.07760100	-3.36897500	-2.06504100
H	-0.47134800	-2.82752000	-2.83977400
H	0.50397000	-4.27247700	-2.51958700
H	-0.62812700	-3.67483600	-1.28893300
Ru	1.03186900	-0.52232300	-0.45879800
O	0.46090500	0.42130500	1.42883700
C	0.63780300	1.56117900	0.90456600
O	1.01102200	1.65503700	-0.29675000
C	0.45165100	2.81468900	1.77328600
F	-0.69007400	2.72514800	2.47633300
F	0.42108900	3.92293000	1.03301400
F	1.47932200	2.89347200	2.63696900
C	-2.14097300	4.22011700	-1.92503900
C	-1.71568500	3.19869100	-2.77929000
C	-1.70115200	1.87927300	-2.33507800
C	-2.14700200	1.56760500	-1.04068300
C	-2.57638700	2.59680600	-0.18655000
C	-2.55926800	3.91955700	-0.62674400
H	-2.14033700	5.25015500	-2.26898600
H	-1.38955200	3.43296400	-3.78810100
H	-2.88514400	2.37186900	0.82948300
H	-2.87199800	4.71391000	0.04393900
C	-2.07157400	0.15227400	-0.59392800
O	-1.05232800	-0.55642300	-0.86436100
N	-3.09432200	-0.42736700	0.06261700
C	-4.45202600	0.13129600	0.17668500
H	-5.17187100	-0.64991700	-0.07893000
H	-4.64574500	0.45829900	1.20317200
H	-4.57604200	0.97009300	-0.50564900
C	-2.89984100	-1.73983100	0.64662200
C	-2.17522400	-1.85970600	1.83452700
C	-3.47485400	-2.86011400	0.04248900

C	-2.02173100	-3.11917500	2.41770500
H	-1.73148800	-0.97865600	2.28771000
C	-3.31855000	-4.11551900	0.63361800
H	-4.03597000	-2.75227700	-0.88160900
C	-2.59254300	-4.24632500	1.82054600
H	-1.46883400	-3.21505000	3.34776300
H	-3.76918600	-4.98787700	0.16963000
H	-2.48145600	-5.22233200	2.28372700
H	-1.35810100	1.08257300	-2.98755600

TS1-int

C	-0.97728100	-2.41091900	-3.99189200
C	-0.50738100	-2.47460600	-2.67984200
C	-1.06736200	-1.65904200	-1.67874400
C	-2.10468800	-0.74882400	-2.03766900
C	-2.54357800	-0.65909200	-3.35648800
C	-1.98599200	-1.50334000	-4.32565800
H	-0.54987000	-3.05105400	-4.75837600
H	0.29792400	-3.15119300	-2.40986700
H	-1.17772400	-2.16653100	-0.57116300
H	-3.29078300	0.07284600	-3.64710700
H	-2.33557900	-1.43752600	-5.35239100
C	-2.48228700	0.20281200	-0.95480500
O	-1.54346900	0.57075100	-0.17921000
N	-3.70372400	0.73936800	-0.82749200
C	-4.91624000	0.11025600	-1.37252800
H	-5.57336700	-0.14510700	-0.53831700
H	-5.43260300	0.79992600	-2.04857300
H	-4.66200200	-0.81186500	-1.88953000
Pd	0.21983900	-0.46799600	-0.44802100
C	2.91027000	-1.26298700	-1.16916300
O	1.78846000	-1.70493300	-0.71977800
O	3.24667700	-0.12483700	-1.47528500
C	-2.70538500	-2.52691600	1.08952000
O	-3.55984400	-1.85096300	0.49483500
O	-1.54755500	-2.87843700	0.70753400
C	-3.09650100	-2.97651700	2.52463900
C	3.97011800	-2.39556900	-1.26713900
C	-3.92630600	1.70481900	0.22923400
C	-4.04442700	3.05508300	-0.10130600
C	-4.07042900	1.26821300	1.54914800
C	-4.30678300	3.98851100	0.90423100
H	-3.93239600	3.36613000	-1.13637200
C	-4.32844800	2.21006900	2.54578500

H	-3.97245000	0.21123700	1.77705500
C	-4.44794600	3.56583600	2.22739700
H	-4.40310700	5.04107800	0.65230100
H	-4.43596800	1.88052500	3.57525900
H	-4.65216700	4.29173700	3.00973000
F	3.42736400	-3.59878100	-1.51627600
F	4.86249700	-2.13473100	-2.23531800
F	4.64874700	-2.47925800	-0.09679200
F	-3.27888300	-1.87889700	3.30634700
F	-4.26189500	-3.65651500	2.51555000
F	-2.17573900	-3.74686700	3.12155700
C	0.37719800	4.19097400	-2.84717100
C	-0.35115000	4.02733400	-1.66689200
C	0.16865100	3.26216300	-0.62259700
C	1.43514200	2.67571400	-0.75268300
C	2.16412700	2.83196600	-1.94016900
C	1.62903400	3.58523100	-2.98498100
H	-0.03145600	4.78415000	-3.66098200
H	-1.32758500	4.49053100	-1.55579600
H	3.11969800	2.33152300	-2.05080000
H	2.18963400	3.69547500	-3.90902900
C	1.96123800	1.85210000	0.38212200
O	1.37028200	0.81069700	0.76823700
N	3.05861000	2.26205300	1.05157900
C	3.75518800	3.53111300	0.81928800
H	3.90439400	4.03740800	1.77755100
H	4.73568700	3.34688500	0.36654800
H	3.16921300	4.17193100	0.16275300
C	3.62438400	1.41108400	2.07775600
C	4.41504300	0.32273200	1.70734000
C	3.40629700	1.71362000	3.42298900
C	4.98327000	-0.47774900	2.69866300
H	4.56046200	0.09979500	0.65662400
C	3.98631800	0.91373400	4.40836500
H	2.77778600	2.55778200	3.69325000
C	4.77360000	-0.18213000	4.04732800
H	5.58104000	-1.33695100	2.40976000
H	3.81408600	1.14150300	5.45649200
H	5.21676400	-0.80822800	4.81663500
H	-0.40784700	3.10906500	0.28393100
TS2-int			
C	-0.47679000	-2.37590500	-4.09248700
C	-1.58855900	-1.66973200	-4.56487100

C	-2.43837100	-1.00008400	-3.68374100
C	-2.17795400	-1.01936100	-2.31128800
C	-1.05391600	-1.72597100	-1.80276400
C	-0.21682300	-2.39971700	-2.72902000
H	0.17427300	-2.89858600	-4.78650700
H	-1.79584500	-1.63258000	-5.63101600
H	-3.29494100	-0.45376800	-4.06585400
H	-1.15041200	-2.19209400	-0.74268300
H	0.64289800	-2.93480500	-2.34116600
N	-3.12961200	-0.39214300	-1.45055200
C	-2.76371400	0.36266100	-0.38976200
O	-1.56800700	0.59754700	-0.06768700
Pd	0.13573500	-0.42046100	-0.50772400
C	-2.31233200	-2.48487700	1.41203200
O	-3.34114200	-1.91234000	1.00670300
O	-1.28891500	-2.86097700	0.77816200
C	2.87715400	-0.95131100	-1.31647500
O	1.80529000	-1.49358000	-0.85498800
C	4.00537800	-2.00684700	-1.48978800
C	-2.25694100	-2.70772800	2.95154500
O	3.11928600	0.21814200	-1.58977200
C	-4.52926100	-0.84905600	-1.59838600
H	-5.02810900	-0.77612300	-0.63558300
H	-5.06563000	-0.26251800	-2.35057400
H	-4.51223800	-1.89932000	-1.89195700
C	-3.79870500	1.13736500	0.36025500
C	-3.87624100	1.03116700	1.75580000
C	-4.60536000	2.05871300	-0.32251300
C	-4.77715800	1.83380800	2.45406000
H	-3.26918400	0.29582800	2.26940500
C	-5.49350300	2.86780000	0.38653100
H	-4.52725500	2.15357200	-1.40237600
C	-5.58223500	2.75265300	1.77531400
H	-4.85192300	1.73759200	3.53338800
H	-6.11284300	3.58526700	-0.14462200
H	-6.27901700	3.37718200	2.32790300
F	4.64288400	-2.19435800	-0.31069000
F	4.91624500	-1.59564200	-2.38456400
F	3.53202300	-3.19880100	-1.89798300
F	-3.40928200	-3.22341400	3.42526000
F	-1.25695500	-3.50805300	3.35167800
F	-2.07812500	-1.50238200	3.56929500
C	-0.11042500	4.44444700	-2.53368100
C	-0.75961200	4.19577200	-1.32218100

C	-0.15654600	3.38798900	-0.35775700
C	1.11009100	2.83943500	-0.60106000
C	1.76054000	3.08309200	-1.81877800
C	1.14418200	3.88184800	-2.78226800
H	-0.58314900	5.07137900	-3.28508900
H	-1.73891200	4.62397800	-1.12700300
H	2.71950200	2.61666100	-2.01468400
H	1.64457500	4.06154600	-3.72973200
C	1.72881000	1.96606400	0.44794400
O	1.22866200	0.85536400	0.76478200
N	2.81478000	2.40038500	1.11889900
C	3.41878900	3.72718200	0.96286900
H	3.54146300	4.18326300	1.94984800
H	4.40525200	3.63874500	0.49474000
H	2.78371200	4.36366700	0.34919900
C	3.46462500	1.51814600	2.06607100
C	4.33991200	0.53685700	1.59950700
C	3.23667700	1.68467600	3.43299800
C	4.98356700	-0.29574500	2.51529300
H	4.49078300	0.41874200	0.53250700
C	3.89204000	0.85426600	4.34299700
H	2.54213300	2.44594000	3.77734600
C	4.76390700	-0.13628600	3.88509000
H	5.64635700	-1.07478700	2.15103500
H	3.71202900	0.97458400	5.40745400
H	5.26497900	-0.78789800	4.59537000
H	-0.66833500	3.17074200	0.57401500

TS1

C	-0.97728100	-2.41091900	-3.99189200
C	-0.50738100	-2.47460600	-2.67984200
C	-1.06736200	-1.65904200	-1.67874400
C	-2.10468800	-0.74882400	-2.03766900
C	-2.54357800	-0.65909200	-3.35648800
C	-1.98599200	-1.50334000	-4.32565800
H	-0.54987000	-3.05105400	-4.75837600
H	0.29792400	-3.15119300	-2.40986700
H	-1.17772400	-2.16653100	-0.57116300
H	-3.29078300	0.07284600	-3.64710700
H	-2.33557900	-1.43752600	-5.35239100
C	-2.48228700	0.20281200	-0.95480500
O	-1.54346900	0.57075100	-0.17921000
N	-3.70372400	0.73936800	-0.82749200
C	-4.91624000	0.11025600	-1.37252800

H	-5.57336700	-0.14510700	-0.53831700
H	-5.43260300	0.79992600	-2.04857300
H	-4.66200200	-0.81186500	-1.88953000
Pd	0.21983900	-0.46799600	-0.44802100
C	2.91027000	-1.26298700	-1.16916300
O	1.78846000	-1.70493300	-0.71977800
O	3.24667700	-0.12483700	-1.47528500
C	-2.70538500	-2.52691600	1.08952000
O	-3.55984400	-1.85096300	0.49483500
O	-1.54755500	-2.87843700	0.70753400
C	-3.09650100	-2.97651700	2.52463900
C	3.97011800	-2.39556900	-1.26713900
C	-3.92630600	1.70481900	0.22923400
C	-4.04442700	3.05508300	-0.10130600
C	-4.07042900	1.26821300	1.54914800
C	-4.30678300	3.98851100	0.90423100
H	-3.93239600	3.36613000	-1.13637200
C	-4.32844800	2.21006900	2.54578500
H	-3.97245000	0.21123700	1.77705500
C	-4.44794600	3.56583600	2.22739700
H	-4.40310700	5.04107800	0.65230100
H	-4.43596800	1.88052500	3.57525900
H	-4.65216700	4.29173700	3.00973000
F	3.42736400	-3.59878100	-1.51627600
F	4.86249700	-2.13473100	-2.23531800
F	4.64874700	-2.47925800	-0.09679200
F	-3.27888300	-1.87889700	3.30634700
F	-4.26189500	-3.65651500	2.51555000
F	-2.17573900	-3.74686700	3.12155700
C	0.37719800	4.19097400	-2.84717100
C	-0.35115000	4.02733400	-1.66689200
C	0.16865100	3.26216300	-0.62259700
C	1.43514200	2.67571400	-0.75268300
C	2.16412700	2.83196600	-1.94016900
C	1.62903400	3.58523100	-2.98498100
H	-0.03145600	4.78415000	-3.66098200
H	-1.32758500	4.49053100	-1.55579600
H	3.11969800	2.33152300	-2.05080000
H	2.18963400	3.69547500	-3.90902900
C	1.96123800	1.85210000	0.38212200
O	1.37028200	0.81069700	0.76823700
N	3.05861000	2.26205300	1.05157900
C	3.75518800	3.53111300	0.81928800
H	3.90439400	4.03740800	1.77755100

H	4.73568700	3.34688500	0.36654800
H	3.16921300	4.17193100	0.16275300
C	3.62438400	1.41108400	2.07775600
C	4.41504300	0.32273200	1.70734000
C	3.40629700	1.71362000	3.42298900
C	4.98327000	-0.47774900	2.69866300
H	4.56046200	0.09979500	0.65662400
C	3.98631800	0.91373400	4.40836500
H	2.77778600	2.55778200	3.69325000
C	4.77360000	-0.18213000	4.04732800
H	5.58104000	-1.33695100	2.40976000
H	3.81408600	1.14150300	5.45649200
H	5.21676400	-0.80822800	4.81663500
H	-0.40784700	3.10906500	0.28393100

TS2

C	-0.67060500	-2.49561100	-4.00078800
C	-1.80909600	-1.82837900	-4.46458700
C	-2.60235400	-1.08232200	-3.59366400
C	-2.25683500	-0.97882800	-2.24258400
C	-1.09632000	-1.63461400	-1.74342200
C	-0.32179000	-2.39082200	-2.66135200
H	-0.06497200	-3.08457100	-4.68292300
H	-2.08498200	-1.88567600	-5.51416200
H	-3.48371900	-0.57316500	-3.97007000
H	-1.21073200	-2.13172500	-0.63890400
H	0.56258200	-2.89203300	-2.28374100
N	-3.16717700	-0.28735900	-1.38662400
C	-2.76252900	0.48044800	-0.34939300
O	-1.55861600	0.69184200	-0.04842200
Pd	0.10979600	-0.38262000	-0.48776800
C	-2.34247400	-2.48544400	1.37719900
O	-3.35794300	-1.87036600	1.02025000
O	-1.33109900	-2.84711100	0.70138300
C	2.83155300	-1.03622700	-1.30384500
O	1.74304800	-1.52604200	-0.82591300
C	3.92029800	-2.13560100	-1.45656600
C	-2.25866900	-2.80188300	2.89687400
O	3.11879100	0.11644500	-1.60564900
C	-4.59023900	-0.67316300	-1.51308400
H	-5.07494500	-0.56957200	-0.54599900
H	-5.10670800	-0.06226000	-2.25979000
H	-4.63048900	-1.72364600	-1.80214900
C	-3.76783600	1.26888200	0.42799700

C	-3.84112000	1.11581400	1.81939100
C	-4.55034600	2.23616500	-0.21772900
C	-4.71358700	1.92026300	2.55135900
H	-3.25249600	0.34589200	2.30402600
C	-5.40875300	3.04686200	0.52530000
H	-4.47729300	2.36405000	-1.29463400
C	-5.49315900	2.88648600	1.90994100
H	-4.78495800	1.78926900	3.62724000
H	-6.00904300	3.80078400	0.02362000
H	-6.16701900	3.51276000	2.48831300
F	4.58147300	-2.28976000	-0.28477900
F	4.82206000	-1.79582900	-2.39024500
F	3.40136300	-3.32938800	-1.79774500
F	-3.40727800	-3.33829100	3.35416500
F	-1.25808100	-3.63076300	3.22775300
F	-2.06218200	-1.63640800	3.57618400
C	-0.01424100	4.40515000	-2.65154600
C	-0.63473400	4.24501300	-1.41052200
C	-0.03979200	3.45419400	-0.42712100
C	1.19111000	2.83410100	-0.68098200
C	1.81305300	2.98964800	-1.92761300
C	1.20413900	3.77168600	-2.90951100
H	-0.48082500	5.01864000	-3.41773600
H	-1.58530800	4.73021600	-1.20653100
H	2.74205000	2.46827200	-2.12918800
H	1.68212100	3.88284000	-3.87886000
C	1.79832900	1.97486900	0.38791700
O	1.26967000	0.89089100	0.74227300
N	2.90650700	2.40094300	1.02938000
C	3.55464500	3.69653900	0.80555500
H	3.71189500	4.19122000	1.76882000
H	4.52855900	3.55198600	0.32505500
H	2.93202000	4.32856200	0.17467500
C	3.54741900	1.53386900	1.99588200
C	4.37058100	0.49936900	1.54974300
C	3.36770700	1.76880800	3.36008200
C	5.00979100	-0.31661700	2.48340300
H	4.48579800	0.32950100	0.48542300
C	4.01873900	0.95447300	4.28771900
H	2.71422700	2.57196500	3.68951200
C	4.83838600	-0.08851800	3.85041400
H	5.63180900	-1.13578000	2.13555400
H	3.87657000	1.12925100	5.35041000
H	5.33651300	-0.72681500	4.57476800

H	-0.53121500	3.30649400	0.52914400
TS1_inner			
C	1.70645600	-3.55517300	-2.26258600
C	1.96092500	-2.46766500	-1.42394500
C	0.95501400	-1.90083100	-0.62377900
C	-0.35029700	-2.46652700	-0.70735300
C	-0.60769800	-3.53933300	-1.56918100
C	0.42138400	-4.08990100	-2.33585000
H	2.50660800	-3.97249000	-2.86732100
H	2.96825100	-2.06383300	-1.37599600
H	1.68604200	-1.50433800	0.51427500
H	-1.61584200	-3.92092400	-1.68998700
H	0.21013700	-4.92089700	-3.00246400
C	-1.44035500	-1.67033000	-0.08290700
O	-1.27807300	-0.41494900	-0.02415200
N	-2.59576700	-2.19784900	0.37399300
C	-2.82389500	-3.62930900	0.60143700
H	-3.32426500	-3.75102700	1.56477300
H	-3.46836700	-4.05699000	-0.17533100
H	-1.87583100	-4.16535900	0.62900200
Pd	0.68674000	0.17921400	-0.20325800
C	-0.36055200	2.64397500	-0.99601900
O	0.22230300	2.13561000	0.04348500
O	-0.60354700	2.11495500	-2.06956500
C	3.23936700	-0.20342400	0.84232100
O	2.69226000	0.63669700	0.08547200
O	2.74579500	-1.29927200	1.24730100
C	4.69290400	0.07908900	1.27797900
C	-0.77135800	4.11787000	-0.73861800
C	-3.66375600	-1.29892600	0.75941100
C	-4.35854900	-0.59301600	-0.22472900
C	-4.00548700	-1.16621800	2.10684900
C	-5.40322200	0.25299400	0.14650500
H	-4.07247300	-0.69612400	-1.26680800
C	-5.05636200	-0.32339100	2.46959200
H	-3.44295700	-1.70246400	2.86605000
C	-5.75568000	0.38614300	1.49120200
H	-5.93876900	0.80952700	-0.61679400
H	-5.31907400	-0.21344700	3.51764000
H	-6.56919900	1.04666600	1.77665700
F	0.29769400	4.86958500	-0.40864500
F	-1.34006000	4.66147800	-1.82407300
F	-1.65907100	4.19440600	0.27593200

F	5.03280000	1.35185500	1.07414100
F	4.85860000	-0.21213600	2.57467800
F	5.51371500	-0.70826800	0.55417800
TS2_inner			
C	-2.22853200	-3.20081900	2.46754800
C	-1.22106200	-4.15089200	2.28708800
C	-0.19262400	-3.92089800	1.37168800
C	-0.17324700	-2.73929800	0.62797600
C	-1.20139600	-1.77696500	0.75662900
C	-2.20980900	-2.03163400	1.71177100
H	-3.02063000	-3.37357000	3.19010300
H	-1.22141200	-5.06674000	2.87126000
H	0.61201500	-4.64296500	1.26812400
H	-1.84184400	-1.33673300	-0.37096300
H	-3.00553300	-1.30164100	1.83609500
N	0.95408900	-2.52928700	-0.24884600
C	1.73575200	-1.43414800	-0.05619200
O	1.35430000	-0.48644200	0.68744200
Pd	-0.55356200	0.21488000	0.41543700
C	-3.05491000	0.21611300	-0.89854300
O	-2.41720200	0.96337400	-0.11684600
O	-2.76588500	-0.97537200	-1.21751100
C	0.71404900	2.65017600	1.11276800
O	0.30255600	2.03269900	0.05145600
C	1.61912400	3.84945800	0.72624500
C	-4.36068300	0.77659200	-1.50434400
O	0.50558500	2.38792600	2.28538300
C	1.13291000	-3.50131000	-1.33767700
H	1.81296800	-3.09611500	-2.08552200
H	1.52846000	-4.45488900	-0.97237400
H	0.15918800	-3.68006300	-1.80168800
C	3.08299600	-1.29662800	-0.66550500
C	3.49621100	0.00467800	-1.00453200
C	3.97247700	-2.37310500	-0.81824300
C	4.76799700	0.21090700	-1.53308200
H	2.82318500	0.83986200	-0.83865100
C	5.24953900	-2.15449700	-1.33049600
H	3.68502700	-3.37199800	-0.50578800
C	5.64348200	-0.86543300	-1.69923300
H	5.07867100	1.21559500	-1.80326100
H	5.93918300	-2.98717800	-1.43358900
H	6.63804500	-0.69888700	-2.10364700
F	2.72853900	3.40167100	0.08145600

F	2.02510300	4.53516700	1.80140500
F	0.98882500	4.70444700	-0.10183100
F	-4.41430400	0.50846200	-2.81680300
F	-5.40851800	0.18079200	-0.90390900
F	-4.46082000	2.09441500	-1.32930400

TS3_benzene

C	-2.73326300	-2.47994100	-2.55079300
C	-2.63714000	-1.26323100	-1.87119200
C	-1.46693500	-0.90596400	-1.17516300
C	-0.36001300	-1.80220500	-1.23943600
C	-0.46344100	-3.03142500	-1.89384000
C	-1.65710800	-3.37014600	-2.54108000
H	-3.64498100	-2.73793500	-3.08182800
H	-3.47590100	-0.57191900	-1.89680800
H	-1.08649300	0.33563600	-1.49041900
H	0.35555200	-3.74260800	-1.88695000
H	-1.73885500	-4.32803900	-3.04589800
C	0.81166000	-1.33482900	-0.45180400
O	0.55466700	-0.60425500	0.56100800
N	2.08997500	-1.60154600	-0.75042000
C	2.55319800	-2.23946300	-1.99444900
H	3.45630300	-1.71834200	-2.31805300
H	2.80024500	-3.29378300	-1.83086900
H	1.79791300	-2.15296200	-2.77501300
C	3.13516800	-1.13182900	0.14413800
C	3.74902000	-2.04447200	1.00244200
C	3.54782600	0.20135300	0.09217200
C	4.79310600	-1.61443400	1.82386000
H	3.41444800	-3.07772600	1.02732700
C	4.59019000	0.62134300	0.91900600
H	3.05646800	0.90203700	-0.57601000
C	5.21370000	-0.28386500	1.78171000
H	5.27680100	-2.32011200	2.49250800
H	4.91606300	1.65657400	0.88605600
H	6.02771600	0.04786400	2.41924900
C	-1.97154600	1.00381500	2.83283900
C	-1.44887400	-0.28066500	3.05358500
C	-2.01863900	-1.41659200	2.38446400
C	-3.10469400	-1.24231400	1.50614300
C	-3.62251600	0.07066600	1.25494100
C	-3.04772300	1.18175200	1.90342200
H	-1.49338900	1.87051600	3.27528700
H	-0.56878400	-0.40806400	3.67469600

H	-3.50133200	-2.09137700	0.96134100
H	-4.41861100	0.21467700	0.53357400
Ru	-1.41628900	0.07563000	0.81895200
O	-0.54577900	1.90422000	0.20283200
C	-0.26829500	2.13780900	-1.00099200
O	-0.52350700	1.39576000	-1.98699900
C	0.51982400	3.43360000	-1.30016700
F	0.43276100	4.30105600	-0.29107000
F	0.07433200	4.01036600	-2.41706800
F	1.81683000	3.09913300	-1.47224800
H	-3.38384000	2.18364100	1.65926200
H	-1.58181700	-2.39955300	2.52150700

TS3_p-dimethylbenzene_cf1

C	2.39073700	-2.67404600	2.68039200
C	2.32702600	-1.40673100	2.09458100
C	1.22497900	-1.01613100	1.31072600
C	0.14505100	-1.93913400	1.18931800
C	0.22115900	-3.21887000	1.74391500
C	1.35150600	-3.58565900	2.48262600
H	3.24891800	-2.95328300	3.28511500
H	3.13484300	-0.70034000	2.27015900
H	0.77120300	0.18401800	1.72300000
H	-0.57050000	-3.94473200	1.59234000
H	1.41059900	-4.58096500	2.91273200
C	-0.96622700	-1.42453600	0.34557800
O	-0.64910300	-0.58557100	-0.55816100
N	-2.25715200	-1.75709700	0.49703800
C	-2.80860000	-2.52315400	1.62719800
H	-3.75984800	-2.06528100	1.90554900
H	-2.99400200	-3.56601600	1.34849700
H	-2.13563600	-2.48335500	2.48329600
C	-3.23303300	-1.23146400	-0.44262800
C	-3.73960000	-2.07561800	-1.43133600
C	-3.69091600	0.08142600	-0.31127300
C	-4.71918500	-1.59706000	-2.30380300
H	-3.37198000	-3.09434400	-1.51683500
C	-4.66780000	0.55098000	-1.18976100
H	-3.28317700	0.72959300	0.45846200
C	-5.18312700	-0.28593100	-2.18303900
H	-5.11900100	-2.25005500	-3.07376200
H	-5.02773000	1.57104700	-1.09504200
H	-5.94691700	0.08357200	-2.86074100
C	2.23471400	1.58720700	-2.15643600

C	1.56832600	0.52008800	-2.79232400
C	1.87556500	-0.83926600	-2.46011100
C	2.87910600	-1.17411000	-1.52264000
C	3.50722200	-0.08059400	-0.83571000
C	3.19331500	1.26301800	-1.13613900
H	0.76850800	0.72778400	-3.49485900
H	4.21622500	-0.29202400	-0.04199300
Ru	1.31373500	0.18515700	-0.56234700
O	0.33275300	1.91526000	0.18033900
C	-0.04746100	2.00758600	1.37423600
O	0.14070300	1.15743600	2.28608300
C	-0.88294800	3.25442400	1.74094100
F	-0.59410200	4.27939100	0.93408900
F	-0.67481200	3.61830200	3.00589400
F	-2.18679900	2.93965100	1.58813500
H	3.65959500	2.06204100	-0.56928700
H	1.29774400	-1.63301200	-2.92367600
C	3.25814500	-2.60243300	-1.24283800
H	2.44611500	-3.28691300	-1.50340500
H	4.13406300	-2.87693200	-1.84397300
H	3.51377500	-2.75170600	-0.19063500
C	1.88117500	3.02085400	-2.43344400
H	1.60115600	3.53614600	-1.50908000
H	2.74575300	3.54073900	-2.86361600
H	1.04782100	3.09860800	-3.13556800

TS3_p-dimethylbenzene_cf2

C	2.01834600	-2.51240700	3.09116000
C	2.13357100	-1.36294200	2.30571300
C	1.07978600	-0.93442800	1.47722600
C	-0.13523000	-1.67786100	1.52028400
C	-0.24423100	-2.84334000	2.28300700
C	0.84072800	-3.26303100	3.06000300
H	2.84478400	-2.82771100	3.72168800
H	3.05089800	-0.78079600	2.34800000
H	0.82862500	0.38445000	1.64948300
H	-1.14659400	-3.44505100	2.26324000
H	0.75840200	-4.17159700	3.64895500
C	-1.17439400	-1.14492700	0.59958400
O	-0.75284400	-0.54879000	-0.444404500
N	-2.49626200	-1.22383300	0.81314200
C	-3.12578600	-1.67809400	2.06451400
H	-3.97280800	-1.02002100	2.26857100
H	-3.49765500	-2.70416400	1.97275700

H	-2.42225500	-1.61347400	2.89396200
C	-3.40577200	-0.72027600	-0.20188900
C	-4.10177900	-1.63328900	-0.99497800
C	-3.61524500	0.65437700	-0.33209400
C	-5.02053500	-1.16252000	-1.93527900
H	-3.92740500	-2.69920400	-0.87748800
C	-4.53303600	1.11473500	-1.27666100
H	-3.06312200	1.35412600	0.28767700
C	-5.23618200	0.20958600	-2.07591700
H	-5.56691200	-1.86843700	-2.55354300
H	-4.70005000	2.18217100	-1.38495000
H	-5.95282600	0.57393200	-2.80587000
C	2.17229500	0.53494300	-2.57845000
C	1.48301000	-0.67254200	-2.76623000
C	1.80116900	-1.84598400	-1.99140600
C	2.82582700	-1.73114400	-1.02748500
C	3.51380600	-0.49119800	-0.81544800
C	3.19862400	0.65638800	-1.57731400
H	1.85414400	1.42025200	-3.11941500
H	0.64733900	-0.70568900	-3.45818600
H	3.04961000	-2.57540900	-0.38434100
H	4.25480500	-0.42104700	-0.02643600
Ru	1.31609800	-0.14121300	-0.58725300
O	0.66595800	1.84928300	-0.20490600
C	0.32460500	2.21988400	0.94542400
O	0.37866800	1.53113300	2.00156400
C	-0.28252700	3.63540100	1.06940400
F	0.16516300	4.43678600	0.09958800
F	0.00024100	4.17811700	2.25338500
F	-1.62306600	3.52355900	0.95200200
C	1.04410900	-3.12844700	-2.20186900
H	-0.01423700	-2.93302400	-2.39847500
H	1.45202500	-3.66411200	-3.06822600
H	1.12332300	-3.78505900	-1.33137900
C	3.87234900	1.98003900	-1.34050300
H	4.59761200	2.17574900	-2.14007500
H	3.14318900	2.79573300	-1.34151300
H	4.40828500	1.99188800	-0.38775000

TS3_p-dimethylbenzene_cf3

C	2.37072200	-2.23262100	3.07280100
C	2.36641800	-1.11824100	2.23037000
C	1.24305000	-0.79429300	1.44758400
C	0.08221600	-1.60678500	1.60034600

C	0.09194400	-2.73863300	2.41958100
C	1.24429000	-3.05472300	3.14661200
H	3.25033700	-2.46441100	3.66659600
H	3.24310000	-0.47690700	2.19512400
H	0.93031900	0.51074500	1.58099100
H	-0.77026300	-3.39389900	2.48273200
H	1.25409100	-3.93727000	3.77912000
C	-1.04457300	-1.18232300	0.72938000
O	-0.72928000	-0.60811500	-0.36344000
N	-2.34223000	-1.33628800	1.03085800
C	-2.86144200	-1.76132800	2.34189600
H	-3.73662600	-1.14849200	2.56690400
H	-3.16832500	-2.81252500	2.32650800
H	-2.11399100	-1.60628800	3.11934400
C	-3.34437200	-0.94192100	0.05575700
C	-4.00770100	-1.93399600	-0.66748200
C	-3.67165700	0.40664100	-0.10206100
C	-5.01342300	-1.56977300	-1.56513300
H	-3.74150100	-2.97806400	-0.52801500
C	-4.67596200	0.76028700	-1.00365300
H	-3.14431600	1.16855500	0.46381100
C	-5.34739800	-0.22465000	-1.73287000
H	-5.53568500	-2.33749000	-2.12815300
H	-4.93554300	1.80669300	-1.13277300
H	-6.13211200	0.05641700	-2.42885100
C	1.74347400	0.38057700	-2.84877900
C	1.28434300	-0.95174300	-2.77410800
C	1.94805300	-1.84268300	-1.85994600
C	3.03904600	-1.39764400	-1.08352200
C	3.52093800	-0.04786600	-1.15995600
C	2.82323500	0.82695700	-2.02553500
H	1.21193200	1.09901200	-3.46317900
H	3.48748300	-2.07796300	-0.36717400
Ru	1.28998300	-0.07430000	-0.66564400
O	0.51326600	1.87066000	-0.31208000
C	0.23185500	2.27078000	0.84432600
O	0.42962700	1.64622400	1.92282800
C	-0.48470100	3.63478900	0.96124600
F	-0.31593400	4.36854200	-0.13995500
F	-0.03884600	4.31643900	2.01766900
F	-1.80458500	3.39827200	1.12415800
H	3.08487100	1.88061500	-2.03508500
H	1.58455100	-2.85821800	-1.74286600
C	4.71674700	0.41435400	-0.37050700

H	4.62558900	1.46590300	-0.08369900
H	4.86125100	-0.18350400	0.53289000
H	5.62284600	0.31202600	-0.98103600
C	0.09503100	-1.42281900	-3.56289500
H	-0.60138700	-1.97718400	-2.92672000
H	-0.44298200	-0.58581900	-4.01394600
H	0.42730200	-2.09222400	-4.36619400

TS3_cf2

C	0.80459100	-3.13433600	3.12535800
C	1.24969100	-2.00511800	2.43366400
C	0.40544400	-1.30568600	1.55115300
C	-0.94339200	-1.75158600	1.44213300
C	-1.38460000	-2.89573200	2.11206300
C	-0.50251800	-3.59166900	2.94537600
H	1.47502700	-3.66110100	3.79846700
H	2.26458300	-1.65047700	2.59577800
H	0.46335100	0.02933600	1.80799200
H	-2.39282000	-3.27233900	1.97574800
H	-0.84333700	-4.48462500	3.46071300
C	-1.74400000	-0.96334700	0.46761300
O	-1.10469200	-0.44660500	-0.50495800
N	-3.06450800	-0.74819900	0.56752700
C	-3.88876000	-1.08596400	1.74039900
H	-4.58042400	-0.25836400	1.91034400
H	-4.47261500	-1.99634700	1.56773800
H	-3.26490700	-1.21052600	2.62491100
C	-3.74590600	-0.01841300	-0.48753800
C	-4.56716500	-0.72138900	-1.36999300
C	-3.62553800	1.37080100	-0.56691600
C	-5.27767300	-0.02295400	-2.34836800
H	-4.65055500	-1.80177300	-1.29113700
C	-4.33665900	2.05898200	-1.55026400
H	-2.98084600	1.90588700	0.12347400
C	-5.16310300	1.36544900	-2.43826300
H	-5.92059100	-0.56460500	-3.03566200
H	-4.24723400	3.13895700	-1.61875000
H	-5.71864700	1.90744300	-3.19771000
C	2.32874600	0.14110700	-2.17177400
C	1.35581400	-0.76238600	-2.62980500
C	1.20029600	-2.05957200	-2.02274400
C	2.05017100	-2.38576700	-0.94409800
C	3.01624100	-1.44479400	-0.46125300
C	3.18769200	-0.17560700	-1.06430500

H	2.35724500	1.13687900	-2.59869100
H	0.66727000	-0.45517600	-3.41040700
H	1.92152100	-3.33042700	-0.42731500
H	3.61236000	-1.70047400	0.40865100
Ru	1.01082600	-0.47515800	-0.42289400
O	0.70872700	1.57885700	0.04477300
C	0.40984000	1.95659500	1.20385800
O	0.27446400	1.22077800	2.22067100
C	0.12956800	3.46517100	1.38079900
F	0.90308400	4.18716500	0.56238900
F	0.33791100	3.85491000	2.63710300
F	-1.16257000	3.69163700	1.06361900
C	0.13986800	-3.00455300	-2.51608200
H	-0.79170000	-2.47152600	-2.72840000
H	0.47377500	-3.48040800	-3.44667100
H	-0.06433500	-3.79373400	-1.78761300
C	4.26859700	0.77004700	-0.56198000
H	4.33273100	0.62369400	0.52473400
C	5.62349900	0.34803700	-1.17532600
H	5.61010200	0.45222700	-2.26649600
H	6.42230000	0.98813900	-0.78708900
H	5.87494600	-0.69089100	-0.93634500
C	3.98996600	2.25745500	-0.82742500
H	3.01359200	2.57269300	-0.44924400
H	4.75783800	2.86201300	-0.33476500
H	4.03849200	2.49355900	-1.89719500

TS3_cf3

C	2.07925700	-0.56322400	3.88986300
C	1.96286100	0.29188000	2.79140100
C	0.95401300	0.11204900	1.82654600
C	0.01491300	-0.93655600	2.04638900
C	0.14445400	-1.81052700	3.12874500
C	1.18538600	-1.62528000	4.04454300
H	2.86732200	-0.40768000	4.62115200
H	2.65743500	1.12237300	2.68966800
H	0.31874400	1.28319900	1.58545600
H	-0.53168400	-2.64909700	3.25753900
H	1.28925400	-2.30686900	4.88345300
C	-0.99075000	-1.05831800	0.95810600
O	-0.61476100	-0.69621800	-0.20364700
N	-2.24835400	-1.49350500	1.12825600
C	-2.89315000	-1.73113800	2.43054900
H	-3.91099300	-1.33963700	2.37460800

H	-2.94521200	-2.80112200	2.65840800
H	-2.35866700	-1.21071700	3.22467100
C	-3.10841800	-1.63511100	-0.03391500
C	-3.37144600	-2.91415500	-0.52585100
C	-3.70245400	-0.50705900	-0.60403300
C	-4.24125000	-3.06607800	-1.60768100
H	-2.90195300	-3.77988700	-0.06716400
C	-4.56744300	-0.66919100	-1.68652500
H	-3.48563400	0.48263300	-0.21388200
C	-4.83863000	-1.94532400	-2.18714700
H	-4.45166000	-4.05912500	-1.99326300
H	-5.03191500	0.20316000	-2.13630700
H	-5.51677700	-2.06545400	-3.02669800
C	2.04837900	0.70439900	-2.45106700
C	1.90001800	-0.67825400	-2.25685700
C	2.51759800	-1.35459700	-1.14521500
C	3.25231600	-0.55635600	-0.23937800
C	3.39369200	0.85728800	-0.42016800
C	2.79238500	1.50894600	-1.52026300
H	1.50979700	1.19079300	-3.25788200
H	1.25174200	-1.23178500	-2.92646400
H	3.67556300	-1.01742300	0.64710900
H	3.92957200	1.44171100	0.32007300
Ru	1.21410600	0.35348000	-0.37000200
O	-0.11266000	2.00331900	-0.62461200
C	-0.65680700	2.56729500	0.35640200
O	-0.48374600	2.28394900	1.57384600
C	-1.68805300	3.67316800	0.03891000
F	-1.43162900	4.24422400	-1.14096600
F	-1.69663700	4.60981500	0.98705800
F	-2.90925600	3.09948300	-0.01563200
C	2.43823200	-2.86003400	-0.95104700
H	2.45357700	-3.03744900	0.13238300
C	2.87430200	2.99908000	-1.70627700
H	3.55697700	3.23245400	-2.53268400
H	1.89308200	3.41578600	-1.95275900
H	3.24898300	3.49550800	-0.80722900
C	1.16647200	-3.50471300	-1.52309700
H	1.15999000	-3.48700400	-2.61927000
H	1.12557800	-4.55665000	-1.22305400
H	0.25864100	-3.00826700	-1.16736900
C	3.70443100	-3.51031000	-1.55366700
H	4.62013700	-3.11062100	-1.10519200
H	3.68630200	-4.59149300	-1.38152200

H	3.75479000	-3.34328200	-2.63590600
TS4_benzene			
C	2.71773100	-2.67862800	2.32363900
C	1.57319300	-3.44117500	2.57479900
C	0.32892500	-3.00439300	2.12403300
C	0.22191000	-1.81404600	1.39685200
C	1.36678200	-1.03810800	1.07304300
C	2.60507900	-1.50837100	1.58333000
H	3.68199400	-2.99414200	2.71044000
H	1.64352300	-4.36721100	3.13763000
H	-0.55614900	-3.59390500	2.33987200
H	1.16007500	0.22229900	1.50759100
H	3.49629200	-0.90831300	1.42270600
N	-1.10990800	-1.37036200	1.07777100
C	-1.45580100	-0.99565500	-0.17690200
O	-0.59522900	-0.76082800	-1.07196900
C	-2.06513400	-1.32564400	2.20782800
H	-2.88915800	-0.65882800	1.96004200
H	-2.46719700	-2.31346400	2.44715400
H	-1.53671200	-0.93365000	3.07933600
C	-2.88032300	-0.87652400	-0.57874500
C	-3.25683900	0.23072400	-1.35690400
C	-3.82169500	-1.87662200	-0.28445000
C	-4.57014000	0.35104500	-1.80417200
H	-2.52063400	0.99318400	-1.59014200
C	-5.12728300	-1.76225900	-0.75681500
H	-3.52869200	-2.75443200	0.28346700
C	-5.50423100	-0.64548400	-1.50792800
H	-4.86437100	1.21754300	-2.38842500
H	-5.84892900	-2.54442100	-0.54208100
H	-6.52528400	-0.55485300	-1.86654800
C	1.92770200	1.18921800	-2.75610000
C	1.56917500	-0.10919000	-3.14412400
C	2.19326300	-1.24641900	-2.53039600
C	3.19190700	-1.05865600	-1.55593800
C	3.55546800	0.26382900	-1.14406300
C	2.89959200	1.37231600	-1.71811400
H	1.40219300	2.04703400	-3.16037900
H	0.75694100	-0.26049800	-3.84688200
H	3.63469600	-1.91866300	-1.06718600
H	4.29034100	0.41475200	-0.36193900
Ru	1.33025600	0.00894400	-0.87631000
O	0.25704600	1.68603600	-0.09355300

C	0.26427300	1.98710600	1.12752100
O	0.78333500	1.31459000	2.05972400
C	-0.49805000	3.27351700	1.52336100
F	-0.43608200	4.18055500	0.54349800
F	-0.00238300	3.80108200	2.64186500
F	-1.78850600	2.94551800	1.72785100
H	3.10997200	2.37177900	-1.35256800
H	1.86766200	-2.24744800	-2.78996400

TS4_p-dimethylbenzene_cf1

C	2.22577900	-2.95723200	2.47152500
C	1.05081400	-3.70799500	2.56049900
C	-0.13720800	-3.20944300	2.02929300
C	-0.15701200	-1.96900900	1.38096700
C	1.02987100	-1.20740100	1.20323400
C	2.20238200	-1.74065100	1.79889900
H	3.14255900	-3.31538300	2.93028400
H	1.04966900	-4.67054400	3.06333200
H	-1.04881200	-3.78996100	2.12572200
H	0.84053800	0.03924500	1.73065600
H	3.11108800	-1.14716400	1.77035200
N	-1.45206600	-1.46859300	0.99796700
C	-1.69363200	-0.94734700	-0.22926800
O	-0.77014400	-0.63504500	-1.02976400
C	-2.50273800	-1.53372400	2.03889700
H	-3.28908600	-0.81755000	1.80702100
H	-2.94540000	-2.53008000	2.11798600
H	-2.04657100	-1.26912700	2.99498600
C	-3.08428900	-0.74625600	-0.71573400
C	-3.38996200	0.46251400	-1.36206700
C	-4.05328200	-1.75946100	-0.63444400
C	-4.66314900	0.66632100	-1.88876400
H	-2.63157000	1.23579000	-1.43211600
C	-5.31671200	-1.55872400	-1.18668400
H	-3.81311600	-2.71131200	-0.17020500
C	-5.62516300	-0.34402300	-1.80505500
H	-4.90369600	1.60932300	-2.37013500
H	-6.05860100	-2.34988600	-1.13743500
H	-6.61394400	-0.18715100	-2.22589900
C	2.20264400	1.50647100	-2.07732700
C	1.56065500	0.51679600	-2.84774000
C	1.81754000	-0.87081300	-2.61671100
C	2.76944600	-1.31383400	-1.66797900
C	3.40824800	-0.29863900	-0.88002800

C	3.11856600	1.06957000	-1.05828600
H	0.79920600	0.80291100	-3.56511100
H	4.10420400	-0.59215700	-0.10228200
Ru	1.18812300	-0.01425700	-0.65902000
O	0.18098400	1.67586300	0.19662200
C	0.16023900	1.89875500	1.43271200
O	0.52306200	1.10088200	2.34053500
C	-0.37054900	3.28913000	1.85092500
F	0.30207400	4.23897400	1.17786600
F	-0.22808700	3.49889500	3.15677600
F	-1.67161200	3.37602400	1.52950600
H	3.58444300	1.80424600	-0.40933100
H	1.23698900	-1.60680100	-3.16439200
C	3.10458200	-2.77071500	-1.50043200
H	2.30149900	-3.40821100	-1.88033500
H	4.01645400	-3.00866800	-2.06255000
H	3.27992900	-3.02389700	-0.45154600
C	1.88430100	2.96723400	-2.22912000
H	1.57140500	3.39808500	-1.27250200
H	2.77454300	3.50962800	-2.56989700
H	1.08451500	3.12834900	-2.95583200

TS4_p-dimethylbenzene_cf2

C	1.88939400	-2.67418000	3.01474700
C	0.61771800	-3.18098100	3.29676300
C	-0.50670600	-2.61833000	2.69585400
C	-0.36621300	-1.56044100	1.79075900
C	0.91054400	-1.05116300	1.43581600
C	2.01946200	-1.63622000	2.09961900
H	2.76452000	-3.08274700	3.51110000
H	0.49633600	-4.00222100	3.99688600
H	-1.49168000	-3.00723500	2.93312500
H	0.91717400	0.30023900	1.65955900
H	3.01011500	-1.23236000	1.91160000
N	-1.58420900	-0.96086700	1.30800300
C	-1.80078200	-0.75227500	-0.01246900
O	-0.87354600	-0.82350800	-0.86737200
C	-2.56892700	-0.57512000	2.34263300
H	-3.25476400	0.16515300	1.93432400
H	-3.14583900	-1.43120600	2.70231200
H	-2.02291100	-0.13609600	3.18029900
C	-3.16222400	-0.45690800	-0.52998700
C	-3.29647700	0.56245600	-1.48708400
C	-4.28189300	-1.22031000	-0.16129100

C	-4.54478500	0.83611500	-2.04078200
H	-2.42433800	1.14069500	-1.77489900
C	-5.52265700	-0.95807100	-0.73848300
H	-4.17986300	-2.03489300	0.54952300
C	-5.65678900	0.07489100	-1.67025900
H	-4.65004400	1.63819400	-2.76496400
H	-6.38322400	-1.56039700	-0.46392400
H	-6.62735000	0.28316100	-2.11076400
C	2.05660600	0.48432600	-2.56949500
C	1.47765500	-0.76107600	-2.84437600
C	1.82876900	-1.93599800	-2.08770500
C	2.79265200	-1.79000600	-1.06684500
C	3.38307600	-0.51686500	-0.77805100
C	3.01248800	0.63760100	-1.50370500
H	1.70844200	1.36596100	-3.09793500
H	0.68484600	-0.82847200	-3.58260500
H	3.04451700	-2.64449600	-0.44840100
H	4.09170600	-0.42562600	0.03773200
Ru	1.14994900	-0.33212800	-0.64415900
O	0.33767300	1.61087700	-0.20067400
C	0.41559400	2.10951200	0.94975100
O	0.75000500	1.50426400	2.00646500
C	0.10957700	3.62162600	1.04703900
F	1.09955400	4.29397800	0.42806600
F	0.03295900	4.03050700	2.31106400
F	-1.04570000	3.89378600	0.42514600
C	1.16631900	-3.25430000	-2.37912600
H	1.29475300	-3.95705600	-1.55177000
H	0.09554200	-3.12258500	-2.56114500
H	1.60779900	-3.70289100	-3.27791600
C	3.57528800	1.99520100	-1.18021400
H	4.27364000	2.30521700	-1.96733600
H	2.78346200	2.74808000	-1.12091200
H	4.11835700	1.98687900	-0.23140000

TS4_p-dimethylbenzene_cf3

C	1.88890800	-2.67432400	3.01501800
C	0.61705000	-3.18049200	3.29735000
C	-0.50721400	-2.61749800	2.69645800
C	-0.36638100	-1.55988100	1.79110800
C	0.91054200	-1.05120500	1.43590200
C	2.01930500	-1.63662000	2.09964300
H	2.76392900	-3.08317600	3.51132000
H	0.49541200	-4.00151600	3.99768200

H	-1.49232400	-3.00593900	2.93392600
H	0.91784700	0.30022600	1.65934100
H	3.01011400	-1.23324300	1.91140500
N	-1.58418800	-0.95998000	1.30824700
C	-1.80087100	-0.75218500	-0.01233700
O	-0.87369700	-0.82432000	-0.86723900
C	-2.56850600	-0.57314900	2.34284100
H	-3.25429600	0.16693800	1.93412300
H	-3.14550400	-1.42880700	2.70339800
H	-2.02214600	-0.13356100	3.17999200
C	-3.16226200	-0.45676100	-0.52993300
C	-3.29621500	0.56174000	-1.48799500
C	-4.28221800	-1.21930600	-0.16033300
C	-4.54448000	0.83541700	-2.04177400
H	-2.42386400	1.13931400	-1.77649300
C	-5.52295300	-0.95707100	-0.73758900
H	-4.18044700	-2.03325400	0.55124500
C	-5.65676700	0.07504800	-1.67034600
H	-4.64949200	1.63684100	-2.76671700
H	-6.38374700	-1.55874700	-0.46231800
H	-6.62730300	0.28332400	-2.11090400
C	1.47738000	-0.76159700	-2.84435200
C	1.82870800	-1.93637000	-2.08755500
C	2.79262800	-1.79011200	-1.06676900
C	3.38288000	-0.51684600	-0.77816100
C	3.01210000	0.63746600	-1.50396100
C	2.05617800	0.48391400	-2.56967100
H	0.68454200	-0.82920300	-3.58253100
H	4.09150800	-0.42537900	0.03760200
Ru	1.14974900	-0.33244800	-0.64419300
O	0.33713600	1.61046900	-0.20066700
C	0.41601100	2.10938100	0.94957500
O	0.75130200	1.50435200	2.00613400
C	0.11026400	3.62156000	1.04677500
F	1.09988500	4.29363300	0.42689800
F	0.03469900	4.03071400	2.31077300
F	-1.04542800	3.89382300	0.42571300
H	1.70786600	1.36542800	-3.09821500
H	3.04464600	-2.64449300	-0.44823600
C	3.57478300	1.99517700	-1.18073600
H	4.27286900	2.30521600	-1.96808500
H	2.78288300	2.74796200	-1.12129600
H	4.11812200	1.98700800	-0.23207700
C	1.16633600	-3.25477100	-2.37870700

H	1.60735200	-3.70320000	-3.27780400
H	1.29538400	-3.95757900	-1.55149300
H	0.09542600	-3.12321000	-2.56006000

TS4_cf2

C	0.85793600	-3.43101000	2.79734100
C	-0.48143400	-3.83040900	2.77656300
C	-1.43220000	-3.04948100	2.12251300
C	-1.04796600	-1.87684000	1.46126100
C	0.31149300	-1.47150800	1.40039700
C	1.23269700	-2.27912400	2.11597100
H	1.59459200	-4.01088200	3.34533900
H	-0.79271000	-4.73713300	3.28678200
H	-2.47329200	-3.35546500	2.13241800
H	0.39583200	-0.17958800	1.85522800
H	2.27104900	-1.96330800	2.16065800
N	-2.10999600	-1.05602600	0.93869500
C	-2.07640400	-0.53931600	-0.31244500
O	-1.03474800	-0.54652300	-1.02543600
C	-3.22968400	-0.78233500	1.86791700
H	-3.74966800	0.12120100	1.55464400
H	-3.94525400	-1.60794300	1.90459400
H	-2.81068000	-0.62803300	2.86414000
C	-3.29449700	0.05010200	-0.92982300
C	-3.16708500	1.28511800	-1.58608500
C	-4.52274100	-0.63002600	-0.95002700
C	-4.26906100	1.84797400	-2.22577000
H	-2.21134600	1.79943300	-1.57233100
C	-5.61368800	-0.07316500	-1.61448900
H	-4.61881100	-1.60158300	-0.47432900
C	-5.49018100	1.16848600	-2.24397500
H	-4.17471200	2.81260600	-2.71506400
H	-6.55811900	-0.60797900	-1.64306300
H	-6.34521300	1.60420200	-2.75240700
C	3.11742700	0.20028200	-0.98961100
C	2.28943700	0.34335400	-2.15580800
C	1.53932900	-0.73519000	-2.64704400
C	1.57983900	-2.03028200	-2.02007600
C	2.39995900	-2.17096000	-0.87956800
C	3.15607500	-1.06929500	-0.36694300
H	2.17278900	1.31856800	-2.61279900
H	2.40826400	-3.11512900	-0.34615200
Ru	0.98306700	-0.49547300	-0.47338600
O	0.40715600	1.47435200	0.18414300

C	0.21526700	1.75977300	1.39076400
O	0.25074100	0.95722000	2.36650200
C	-0.15886400	3.22896200	1.69354900
F	0.56784900	4.06189900	0.93583200
F	0.03134900	3.52894900	2.97662000
F	-1.46010700	3.39999700	1.39120800
H	3.75372100	-1.20027600	0.52891100
H	0.85117500	-0.57153800	-3.47050800
C	0.75839200	-3.16819300	-2.56072700
H	-0.22982100	-2.82334400	-2.87928400
H	1.25848400	-3.60607600	-3.43380500
H	0.62892100	-3.95724400	-1.81515300
C	3.97916200	1.33273700	-0.45120700
H	3.98733600	1.23201400	0.64247400
C	5.42816800	1.12583800	-0.95179800
H	6.07734000	1.90257700	-0.53503100
H	5.82954100	0.15180000	-0.65269000
H	5.48045600	1.19466500	-2.04455900
C	3.48003900	2.74274600	-0.79939200
H	2.44629300	2.90660500	-0.48515100
H	4.10859100	3.48244700	-0.29376100
H	3.55478000	2.94497400	-1.87452300

TS4_cf3

C	2.41290800	-1.50370800	3.24040500
C	1.52495000	-2.57345000	3.37627800
C	0.33000000	-2.58222100	2.65875300
C	0.02554700	-1.53547100	1.78142500
C	0.93188400	-0.46328400	1.56063100
C	2.11396400	-0.48274700	2.34478000
H	3.32130300	-1.46562700	3.83422500
H	1.74764900	-3.39064800	4.05594900
H	-0.36433500	-3.40617100	2.78806400
H	0.28094900	0.71272200	1.82234700
H	2.79336600	0.36156800	2.27951400
N	-1.28880800	-1.55652000	1.19259400
C	-1.47951400	-1.38557800	-0.13795700
O	-0.57581100	-0.93880000	-0.89678800
C	-2.41447000	-1.74966900	2.13326300
H	-3.33750000	-1.40303100	1.67185000
H	-2.53624000	-2.79657500	2.42326900
H	-2.21352900	-1.15405800	3.02638200
C	-2.76767900	-1.75533800	-0.78046800
C	-3.30706100	-0.87644600	-1.73398200

C	-3.39804700	-2.98507800	-0.52957300
C	-4.48341900	-1.21032900	-2.40060300
H	-2.80690800	0.06612300	-1.93190500
C	-4.56102900	-3.32375900	-1.21797900
H	-2.96650200	-3.68726000	0.17741400
C	-5.10908400	-2.43378500	-2.14568700
H	-4.90963000	-0.52044600	-3.12257900
H	-5.03737700	-4.28178000	-1.03345300
H	-6.02108300	-2.69658300	-2.67354200
C	1.56117200	1.99882300	-2.05239800
C	1.44421700	0.74062000	-2.67449000
C	2.14529100	-0.39824100	-2.16628800
C	3.03660200	-0.30903600	-1.07080200
C	3.13147500	0.97422900	-0.43274900
C	2.40142600	2.09058000	-0.88909200
H	0.74824300	0.61064700	-3.49612000
H	3.75480500	1.08063600	0.44838700
Ru	0.95343200	0.42501800	-0.47160800
O	-0.70201200	1.72628400	-0.04167800
C	-0.95293000	2.12605500	1.12238100
O	-0.45347200	1.67425800	2.18991400
C	-1.95698700	3.29689600	1.22207300
F	-1.45998100	4.34896500	0.54494900
F	-2.17462300	3.65676400	2.48400000
F	-3.12044400	2.93684900	0.65930900
H	2.46327200	3.02955100	-0.34824800
H	1.94988200	-1.36395200	-2.61851900
C	3.89123600	-1.46974200	-0.59337100
H	4.03468400	-1.33375300	0.48573100
C	0.76816800	3.19136300	-2.50705500
H	0.20650400	3.62624600	-1.67418700
H	1.44486000	3.96136400	-2.89743200
H	0.06129700	2.92419800	-3.29628500
C	5.27851200	-1.38541200	-1.26900900
H	5.93086900	-2.17528700	-0.88247700
H	5.19559000	-1.51678000	-2.35405700
H	5.76691700	-0.42289100	-1.08091100
C	3.25130000	-2.84825200	-0.80954200
H	3.87404200	-3.61807600	-0.34329300
H	2.25244600	-2.90259000	-0.36404600
H	3.17226300	-3.10197300	-1.87305100
TS3_outer			
C	0.34564200	2.16501200	3.93087300

C	0.89128000	1.72478400	2.72683500
C	0.13769100	0.99550300	1.78607900
C	-1.20059800	0.68924000	2.13333700
C	-1.75607900	1.13320100	3.33982200
C	-0.98470500	1.87142300	4.23808200
H	0.95882100	2.71827700	4.63699000
H	1.94521500	1.88913300	2.52283700
H	0.98305100	0.27007600	1.20736900
H	-2.79893600	0.92981300	3.56584600
H	-1.42116300	2.21132600	5.17316500
C	-2.07619300	0.13347500	1.06762600
O	-1.93945100	0.61479100	-0.09742600
N	-3.06920400	-0.73467600	1.32563400
C	-3.05995300	-1.63578500	2.48776000
H	-2.99259000	-2.66622300	2.12786800
H	-3.97984300	-1.51780300	3.06986400
H	-2.19263100	-1.43446500	3.11315800
C	-3.97748800	-1.09782000	0.25847200
C	-5.22872500	-0.48286600	0.19749900
C	-3.61852800	-2.08491800	-0.66300200
C	-6.13197900	-0.85497800	-0.80030700
H	-5.48778600	0.27996800	0.92653000
C	-4.52675800	-2.44915500	-1.65752300
H	-2.63781900	-2.54407400	-0.60585600
C	-5.78160300	-1.83820900	-1.72749800
H	-7.10696700	-0.37809100	-0.85020300
H	-4.24839600	-3.21040600	-2.38067400
H	-6.48485600	-2.12775400	-2.50353700
C	0.24241200	2.12706800	-2.58390400
C	-0.77890500	2.85891900	-1.94134900
C	-0.53499800	3.58530000	-0.72351800
C	0.75543300	3.46941200	-0.16652600
C	1.79145200	2.69911400	-0.79499000
C	1.56343600	2.02934800	-2.01751600
H	-0.00393500	1.52707900	-3.45323200
H	-1.78873700	2.81872000	-2.33896500
H	0.94993300	3.90608100	0.80724200
H	2.73075600	2.56133900	-0.27451700
C	2.59228000	1.14871600	-2.70541600
H	2.08011600	0.20005400	-2.91226700
C	2.99667000	1.79382200	-4.04930100
H	2.13351600	1.98765300	-4.69657700
H	3.67595600	1.12550400	-4.58882100
H	3.51860500	2.74480200	-3.88711100

C	3.82455800	0.83155500	-1.84961800
H	4.47449600	0.14160600	-2.39790600
H	3.54908000	0.35208200	-0.90636300
H	4.41525100	1.73363700	-1.64075500
C	-1.63037000	4.37206200	-0.05551400
H	-2.60035000	3.88125200	-0.18236800
H	-1.70185100	5.37533300	-0.49519000
H	-1.43931300	4.48498000	1.01545900
Ru	0.00311200	1.39329800	-0.50413300
O	2.47434500	-1.07227000	3.08618400
C	2.74864900	-1.07115500	1.89370700
O	2.25208600	-0.36836400	0.93443900
C	3.84971300	-2.03413400	1.36679000
F	4.41336400	-2.75740300	2.34567800
F	3.34065300	-2.89653200	0.45736400
F	4.84291600	-1.34292400	0.74877800
O	-0.42311300	-1.88249000	0.46926200
C	0.10490600	-1.65163500	-0.61308900
O	0.33739500	-0.53505300	-1.20413800
C	0.49086000	-2.86739700	-1.49760900
F	0.95513100	-3.88321500	-0.76330500
F	-0.63013400	-3.30277900	-2.13935300
F	1.40242500	-2.57654800	-2.44220100

TS4_outer

C	-0.42360800	1.17084900	4.16671700
C	0.83181300	0.66453000	4.52414400
C	1.60762400	0.00221400	3.57615200
C	1.14484600	-0.14123900	2.26292200
C	-0.09041200	0.40304200	1.84670300
C	-0.86198200	1.03606600	2.85639500
H	-1.05403200	1.64630500	4.91336300
H	1.19607300	0.76684400	5.54277900
H	2.57231400	-0.41334300	3.85285200
H	-0.86149400	-0.28591700	1.12239500
H	-1.85831200	1.37958200	2.59281100
N	1.96649100	-0.93744800	1.39268000
C	2.45876600	-0.43610600	0.24817300
O	2.11259800	0.69035300	-0.21475200
C	1.99497100	-2.38201500	1.71942600
H	2.34950600	-2.93688900	0.85374800
H	2.64514800	-2.57446300	2.57902200
H	0.96868300	-2.68622200	1.94322200
C	3.57914600	-1.12863100	-0.45235500

C	3.57372100	-1.19626800	-1.85248600
C	4.68369800	-1.61401000	0.26175000
C	4.65164600	-1.76632300	-2.52552400
H	2.71086100	-0.82803200	-2.39423700
C	5.76801100	-2.16979400	-0.41688700
H	4.70114200	-1.54271600	1.34533400
C	5.75035900	-2.25168700	-1.81057100
H	4.63385800	-1.83530500	-3.60947600
H	6.62398800	-2.53742900	0.14198900
H	6.59099700	-2.69288500	-2.33922400
C	-0.17180600	3.04094700	-1.76248600
C	1.03714300	3.38968900	-1.13043100
C	1.09427800	3.66140500	0.28271100
C	-0.10532900	3.53647100	1.00925000
C	-1.33341800	3.15073500	0.37020700
C	-1.39646300	2.89888300	-1.01713100
H	-0.15869600	2.75030300	-2.80779000
H	1.95972600	3.37285900	-1.70256300
H	-0.08731600	3.64754100	2.08765900
H	-2.21274900	2.98881100	0.98056800
C	-2.64814300	2.42475100	-1.73480800
H	-2.31243300	1.66722500	-2.45282400
C	-3.26392500	3.60582200	-2.51564400
H	-2.54291000	4.06667200	-3.20119100
H	-4.11556100	3.25635400	-3.10893800
H	-3.62512800	4.38458700	-1.83273900
C	-3.68261400	1.74688000	-0.82659700
H	-4.51131600	1.38093600	-1.44173400
H	-3.25768000	0.88504300	-0.30313100
H	-4.11140400	2.44509300	-0.09557200
C	2.40302400	4.00054600	0.94280900
H	3.20745200	3.36854200	0.55363400
H	2.66998000	5.04696200	0.74698600
H	2.34813500	3.85985700	2.02589600
Ru	0.20851700	1.60586800	-0.10497000
O	-1.24332300	-2.71191000	2.11756500
C	-2.04562600	-2.17883500	1.35715100
O	-1.96770000	-1.05302800	0.74009700
C	-3.38902800	-2.89988600	1.05550500
F	-3.56949400	-3.06237400	-0.27176500
F	-4.43205200	-2.16998000	1.52042500
F	-3.45358400	-4.11063300	1.63055300
O	-0.50809000	0.14123000	-1.39586400
C	-0.29933500	-1.12118100	-1.52287100

O	0.58132900	-1.83336800	-1.05826200
C	-1.31243300	-1.75506000	-2.51564700
F	-1.50325000	-3.05363200	-2.26066900
F	-0.81328200	-1.64900200	-3.77639900
F	-2.51023800	-1.14252400	-2.51021800

TS5

C	-0.40304000	-2.68341200	3.47359600
C	-0.97648200	-1.76680400	2.58965200
C	-0.20314300	-1.09524400	1.62295100
C	1.19456000	-1.36880200	1.60296600
C	1.77012800	-2.29335800	2.47816400
C	0.96699600	-2.95274800	3.41213100
H	-1.01985900	-3.18573800	4.21314200
H	-2.03652500	-1.54108200	2.67469300
H	-0.48113500	0.21035000	1.69832000
H	2.82814600	-2.53987600	2.42492800
H	1.41189200	-3.67389900	4.09092300
C	1.93600000	-0.64309700	0.54768800
O	1.28363100	-0.20223700	-0.44748100
N	3.25795500	-0.45319200	0.67173300
C	4.19198900	0.18123000	-0.19686500
C	5.54117200	0.08753600	0.17443000
C	3.82418000	0.87861800	-1.35524400
C	6.52269900	0.68423700	-0.61096200
H	5.82294100	-0.45317600	1.07576100
C	4.82182800	1.46959400	-2.13190500
H	2.78427100	0.96624700	-1.63499000
C	6.16642600	1.37724200	-1.77024300
H	7.56438600	0.60690000	-0.31525800
H	4.53717500	2.01376900	-3.02755500
H	6.93083600	1.84411100	-2.38344800
C	-2.03673200	-0.35418400	-2.34754900
C	-0.94932100	-1.19964700	-2.61224500
C	-0.71307600	-2.38186700	-1.82100500
C	-1.60800200	-2.64550800	-0.76382300
C	-2.70094000	-1.76207800	-0.47520200
C	-2.93809800	-0.60628400	-1.25307500
H	-2.13691500	0.57049200	-2.90708000
H	-0.23723700	-0.92798900	-3.38523900
H	-1.42749100	-3.49260200	-0.11071500
H	-3.32213700	-1.96575000	0.38834900
C	-4.06463900	0.37784400	-0.98383900
H	-3.63901500	1.37966000	-1.12790200

C	-5.17741700	0.17408000	-2.03656500
H	-4.79717200	0.26898400	-3.05944700
H	-5.95993100	0.92701600	-1.89931100
H	-5.63752700	-0.81557900	-1.93543400
C	-4.63428300	0.31141200	0.43941200
H	-5.36187700	1.11646500	0.57869200
H	-3.85499500	0.43503500	1.19998400
H	-5.15972500	-0.63248100	0.62747800
C	0.46204900	-3.27308200	-2.11525500
H	1.34897100	-2.68563100	-2.37174300
H	0.23184500	-3.91913200	-2.97177800
H	0.70066400	-3.91599200	-1.26381000
Ru	-0.81341400	-0.57047500	-0.45463000
O	-0.93776200	1.52987200	-0.20822700
C	-0.84029000	2.06596100	0.92734300
O	-0.59474800	1.47504200	2.01083400
C	-1.09821800	3.58976700	0.96162400
F	-2.38800000	3.80931400	0.64435600
F	-0.85520100	4.10197600	2.16588300
F	-0.32357800	4.20232900	0.05722400
H	3.66088000	-0.78928100	1.53780800

TS6

C	0.78542400	-2.47373200	3.48742000
C	-0.52557100	-2.94917300	3.61120100
C	-1.53102900	-2.45477300	2.78517800
C	-1.22803400	-1.49344100	1.81231500
C	0.09324700	-1.00860900	1.62650700
C	1.07342600	-1.52309700	2.51558200
H	1.56228700	-2.83266100	4.15553100
H	-0.77070700	-3.69025800	4.36612800
H	-2.55230600	-2.81071700	2.90170100
H	0.06151700	0.33491500	1.70776700
H	2.08367100	-1.12723100	2.45092300
N	-2.32633400	-0.97264800	1.08727600
C	-2.33742400	-0.25419700	-0.05937800
O	-1.29997600	0.01738400	-0.71626700
C	-3.64841900	0.22922800	-0.55723200
C	-3.66208000	1.36649300	-1.38172700
C	-4.85896900	-0.41346700	-0.24273100
C	-4.86980500	1.86660500	-1.86076500
H	-2.72513800	1.85486900	-1.62627800
C	-6.06269200	0.08571100	-0.73385100
H	-4.87433900	-1.32833300	0.34496400

C	-6.07050700	1.22948000	-1.53670200
H	-4.87525600	2.75443200	-2.48550800
H	-6.99258900	-0.42189800	-0.49715200
H	-7.01130200	1.61941500	-1.91354100
C	1.82903200	-0.49690700	-2.44191200
C	0.76239500	-1.40423200	-2.53830800
C	0.61216700	-2.49905600	-1.61790100
C	1.57784300	-2.61011900	-0.59238700
C	2.65664200	-1.67809300	-0.47119400
C	2.79523200	-0.60465300	-1.38390700
H	1.87201500	0.35249000	-3.11562700
H	-0.01015500	-1.23473100	-3.28258400
H	1.46585000	-3.38287300	0.16106700
H	3.34550100	-1.77793700	0.35806300
C	3.91451800	0.41812700	-1.30427400
H	3.49040500	1.37022100	-1.64685600
C	5.02699500	0.00605500	-2.29664100
H	4.64542300	-0.10392100	-3.31744600
H	5.81030300	0.77047400	-2.31036200
H	5.48577700	-0.94426000	-2.00048700
C	4.48195900	0.63907000	0.10389300
H	5.22877300	1.43827800	0.07191800
H	3.70253900	0.94256700	0.80989500
H	4.98576100	-0.25387800	0.49235100
C	-0.52099200	-3.48010400	-1.75763400
H	-1.42591100	-2.99351400	-2.13411900
H	-0.24786600	-4.26698900	-2.47192700
H	-0.75283800	-3.96090000	-0.80312100
Ru	0.71084000	-0.55721400	-0.44733800
O	1.01076900	1.52296200	-0.09456700
C	0.59281600	2.11589100	0.93094900
O	-0.01556900	1.58917500	1.90363300
C	0.92833500	3.62104000	1.03438100
F	2.17415100	3.73933300	1.53022800
F	0.07720200	4.25190300	1.84355700
F	0.89144000	4.19487200	-0.17387300
H	-3.22804700	-1.09702300	1.52977100
TS5_no_H			
C	-0.26969700	4.09185000	2.03258400
C	-0.79304400	2.96007700	1.40814300
C	0.01112800	1.82322400	1.16528000
C	1.36308600	1.87698900	1.57384800
C	1.89053500	3.00230700	2.20691200

C	1.07410400	4.11225100	2.42922200
H	-0.90519700	4.95301500	2.22429700
H	-1.84871800	2.93666300	1.14214200
H	-0.62663400	0.77222900	1.75781700
H	2.93395400	2.98761500	2.50797000
H	1.47867000	4.99360600	2.92068300
C	2.24148900	0.69507300	1.27989000
C	-0.69776300	-0.44283000	-2.55734600
C	0.63351400	-0.00812900	-2.61751500
C	0.98631300	1.34317900	-2.27073500
C	-0.06457400	2.20517900	-1.87867700
C	-1.43257600	1.77248700	-1.85495100
C	-1.76781200	0.44323900	-2.16641600
H	-0.92103300	-1.49075600	-2.73161000
H	1.41955800	-0.72317800	-2.83616500
H	0.17243200	3.21114600	-1.54849300
H	-2.19365300	2.46425200	-1.51510700
C	-3.18391200	-0.10682200	-2.10788100
H	-3.10275900	-1.11756100	-1.68658800
C	-3.75097100	-0.23191700	-3.53850500
H	-3.10555900	-0.84229000	-4.17971900
H	-4.74141400	-0.69965100	-3.51412200
H	-3.85314200	0.75512200	-4.00526600
C	-4.13518100	0.69386600	-1.20921000
H	-5.09626200	0.17491000	-1.13265400
H	-3.73235900	0.80672600	-0.19727100
H	-4.33785300	1.69237600	-1.61533500
C	2.41833500	1.80269700	-2.32293900
H	3.09597200	1.00501200	-2.00548500
H	2.68643600	2.08623400	-3.34919200
H	2.58111300	2.67075800	-1.67799800
Ru	-0.11936700	0.44352400	-0.53251900
O	-1.14782500	-1.15179400	0.49649400
C	-1.42286900	-1.07423500	1.71580400
O	-1.18880900	-0.10091300	2.48333000
C	-2.15599200	-2.29619600	2.30893300
F	-3.37175200	-2.40580800	1.73465000
F	-2.32045500	-2.19336300	3.62942200
F	-1.46600000	-3.41762000	2.04527000
N	1.63488300	-0.20330100	0.43840200
O	3.37023200	0.60296100	1.77240800
C	2.34479200	-1.33479700	-0.03903100
C	3.72328100	-1.29834500	-0.33585900
C	1.64671500	-2.53425100	-0.27904400

C	4.36296700	-2.41772300	-0.86868200
H	4.28902500	-0.40272400	-0.11526000
C	2.29570400	-3.64631500	-0.81436400
H	0.59367900	-2.58893800	-0.02717400
C	3.65808000	-3.59693500	-1.11842800
H	5.42702400	-2.36427400	-1.08709500
H	1.73197900	-4.56094500	-0.98336500
H	4.16384800	-4.46575100	-1.53110900

TS6_no_H

C	-0.19647900	4.69069500	-0.39963500
C	0.57653100	3.60740900	0.01895200
C	0.13142200	2.29370600	-0.22441500
C	-1.15973900	2.09570000	-0.79234700
C	-1.95953100	3.18005300	-1.19542300
C	-1.44480400	4.46375500	-1.00271800
H	0.16558700	5.70734700	-0.26977700
H	1.55265000	3.78129500	0.47060700
H	1.13316700	1.76788100	-1.12129200
H	-2.94279200	3.01699200	-1.61375200
H	-2.03861500	5.31758300	-1.32211800
C	0.19438400	-1.49455000	2.10106700
C	-1.06821500	-0.89396200	2.19090100
C	-1.20633400	0.50768200	2.49343800
C	-0.01607700	1.24816700	2.70344200
C	1.27877100	0.63730900	2.62990900
C	1.39955900	-0.72542200	2.28482300
H	0.26893000	-2.52952800	1.78420600
H	-1.95346900	-1.47360500	1.95100300
H	-0.08453100	2.31728300	2.87601000
H	2.16074800	1.25372700	2.75137200
C	2.73811200	-1.42891700	2.11525300
H	2.62743400	-2.09548700	1.24976900
C	3.02047300	-2.30414600	3.35555100
H	2.20753900	-3.01302800	3.54698100
H	3.94251700	-2.87838700	3.21218400
H	3.14348000	-1.68315300	4.25099600
C	3.91874100	-0.49194700	1.82863600
H	4.81613500	-1.08376000	1.62008600
H	3.72832300	0.14595900	0.95975500
H	4.14771700	0.15132300	2.68688000
C	-2.56378700	1.15386000	2.58386100
H	-3.26309800	0.71258700	1.86798000
H	-2.98183300	1.02129200	3.59043000

H	-2.50405500	2.22637600	2.37853800
Ru	0.11345600	0.34783000	0.70876400
O	1.27675300	-0.58832800	-0.86484500
C	1.86692200	0.05147000	-1.75711800
O	1.86310100	1.31000100	-1.93169700
C	2.75647000	-0.76837900	-2.71509700
F	3.93419300	-1.01621200	-2.10357400
F	2.99969200	-0.11634500	-3.85470100
F	2.17853800	-1.94276300	-3.00417400
N	-1.41071200	0.72564000	-0.73795200
C	-2.62926200	0.17368900	-1.04057600
O	-3.60976600	0.82799700	-1.41564000
C	-2.75260300	-1.32361900	-0.91030500
C	-4.02475200	-1.84758600	-0.63593400
C	-1.68181800	-2.20672400	-1.11379900
C	-4.21779500	-3.22418000	-0.52574600
H	-4.85386000	-1.15578200	-0.52492600
C	-1.88083000	-3.58609700	-1.02364200
H	-0.70028900	-1.81679500	-1.35792600
C	-3.14455000	-4.09837700	-0.71879400
H	-5.20660800	-3.61626900	-0.30172800
H	-1.04830300	-4.26241100	-1.20204200
H	-3.29521800	-5.17247800	-0.64540300

TS3_3CO

C	-2.89776500	-2.63855300	-2.21731600
C	-2.80073200	-1.41398900	-1.55107100
C	-1.58072100	-0.97487800	-0.99957000
C	-0.43566000	-1.81539700	-1.16250000
C	-0.53807100	-3.04870300	-1.80393600
C	-1.77331100	-3.45697300	-2.32680800
H	-3.84617100	-2.95796000	-2.63831100
H	-3.68060700	-0.77981300	-1.47737700
H	-1.31800300	0.26729200	-1.37661500
H	0.31431000	-3.71522200	-1.87915200
H	-1.84960400	-4.42100700	-2.82069400
C	0.78648100	-1.32384900	-0.46361200
O	0.60129900	-0.67016300	0.62019300
N	2.03402800	-1.50796700	-0.89997600
C	2.40133200	-2.06248100	-2.21519200
H	3.22474000	-1.46276200	-2.60786900
H	2.74041100	-3.09914700	-2.12112400
H	1.56143500	-2.00624000	-2.90676100
C	3.14289200	-1.03591900	-0.08303000

C	3.83546800	-1.95072000	0.70991800
C	3.52559500	0.30517800	-0.14964000
C	4.93387000	-1.51197600	1.45187300
H	3.52059500	-2.98967700	0.74725900
C	4.62354700	0.73240300	0.59774600
H	2.96895900	1.00519400	-0.76569200
C	5.32780300	-0.17371500	1.39492400
H	5.47989400	-2.21708200	2.07104600
H	4.92844400	1.77353600	0.55505300
H	6.18383700	0.16378600	1.97127600
Ru	-1.35402000	0.02080700	1.00637200
O	-0.60972300	1.88682500	0.26620900
C	-0.50729800	2.12279100	-0.96814400
O	-0.89596100	1.38419800	-1.90933200
C	0.24120400	3.41952100	-1.36097300
F	0.19836800	4.31773600	-0.37878200
F	-0.27232700	3.94666500	-2.47057600
F	1.53051000	3.08792800	-1.59234300
C	-0.82517500	0.72765500	2.78001500
O	-0.48041400	1.12462400	3.78816300
C	-1.92342800	-1.67070700	1.71321900
O	-2.24744000	-2.68885200	2.11546600
C	-3.12495600	0.76211000	1.13637700
O	-4.17588200	1.20806800	1.16305900

TS4_3CO

C	-3.04419400	-2.60014300	-2.01251900
C	-1.94331100	-3.38718000	-2.36110000
C	-0.64952000	-2.98174400	-2.02809800
C	-0.44749400	-1.79402300	-1.32256200
C	-1.54318500	-0.97719800	-0.92633100
C	-2.83875100	-1.42401500	-1.30154500
H	-4.04741100	-2.90517500	-2.29277000
H	-2.08662600	-4.31751600	-2.90257500
H	0.19572800	-3.59803900	-2.31636000
H	-1.30870300	0.26071900	-1.38458800
H	-3.70060400	-0.81292200	-1.04698900
N	0.91749600	-1.38176100	-1.11426700
C	1.39179600	-1.05225700	0.11128900
O	0.62386200	-0.83258100	1.09701600
C	1.75363200	-1.30849900	-2.33652300
H	2.61853500	-0.67576300	-2.14649100
H	2.09605600	-2.29506400	-2.65789400
H	1.14968400	-0.86149400	-3.12894500

C	2.84801800	-0.96779200	0.37179000
C	3.32152000	0.09725200	1.15717400
C	3.73750000	-1.96578300	-0.06268100
C	4.67544200	0.18078100	1.47016500
H	2.62892800	0.85877900	1.50021000
C	5.08583400	-1.88934700	0.27688200
H	3.37355000	-2.81516100	-0.63260100
C	5.55671900	-0.81247300	1.03358300
H	5.04280700	1.01514800	2.05943100
H	5.76787900	-2.67039000	-0.04432800
H	6.61054900	-0.75107200	1.28830200
Ru	-1.28808900	0.05821900	1.03216400
O	-0.27184000	1.75052000	0.18664700
C	-0.32428600	2.02319200	-1.04374100
O	-0.91957000	1.35810600	-1.93270000
C	0.48807900	3.25790800	-1.50359800
F	0.51073200	4.18907000	-0.54884200
F	-0.01980000	3.77613100	-2.61909900
F	1.74927000	2.84717400	-1.74296800
C	-2.97575700	0.96580800	0.92733800
O	-3.97231600	1.51666700	0.83096500
C	-0.86118700	0.86150700	2.80894000
O	-0.58282900	1.30772200	3.81705000
C	-2.07641400	-1.51173700	1.80236000
O	-2.52423100	-2.46521800	2.24145600

TS3_no_cap

C	-3.57736800	-2.72495100	-0.99569300
C	-3.35073800	-1.48899000	-0.38520600
C	-2.04904100	-1.04995800	-0.07997400
C	-0.96464200	-1.88413200	-0.47817100
C	-1.18865500	-3.13256400	-1.06450400
C	-2.49917000	-3.55412900	-1.31242200
H	-4.59102700	-3.04557700	-1.21867800
H	-4.19792900	-0.84730700	-0.15589000
H	-1.87327000	0.22854700	-0.50430100
H	-0.36423700	-3.79511800	-1.30600800
H	-2.67346600	-4.52691100	-1.76234300
C	0.36470300	-1.34508600	-0.08520300
O	0.39610000	-0.62399600	0.96411100
N	1.50021100	-1.54555700	-0.77063400
C	1.58538400	-2.16579600	-2.10342500
H	2.30838100	-1.59566600	-2.69029200
H	1.93228800	-3.20258900	-2.03769900

H	0.61906800	-2.13132100	-2.60558400
C	2.74496000	-1.01037200	-0.24632500
C	3.65499600	-1.88104400	0.35417000
C	3.04068800	0.34548900	-0.40391500
C	4.87989200	-1.38583800	0.80629500
H	3.40822600	-2.93326900	0.46498300
C	4.26579400	0.83103000	0.05392100
H	2.32202600	1.01242800	-0.87030700
C	5.18521900	-0.03188400	0.65607700
H	5.59336000	-2.05908500	1.27192400
H	4.50242500	1.88420200	-0.06393000
H	6.13940600	0.35088200	1.00563300
Ru	-1.44822500	0.00265600	1.78506200
O	-0.86521200	1.85106800	0.89436400
C	-1.03427000	2.06623000	-0.33037700
O	-1.58917300	1.29021800	-1.15794900
C	-0.45365600	3.37887400	-0.90200700
F	-0.26430200	4.28434500	0.05995900
F	-1.25935000	3.89040000	-1.83389900
F	0.73886000	3.09450300	-1.46821900

TS4_no_cap

C	-3.08557900	-3.30176300	-0.69211000
C	-1.97486800	-3.89238500	-1.30086900
C	-0.74737700	-3.23273900	-1.30166600
C	-0.61574500	-1.98884400	-0.67385900
C	-1.70335400	-1.38092400	0.00542300
C	-2.93806900	-2.07665000	-0.05230000
H	-4.05377600	-3.79245700	-0.72441100
H	-2.06480600	-4.85742200	-1.79073400
H	0.10595000	-3.69097200	-1.79119200
H	-1.88800400	-0.10815600	-0.49106500
H	-3.81500700	-1.61522500	0.39220800
N	0.65323100	-1.32305900	-0.82690700
C	1.32427700	-0.81223800	0.23240300
O	0.78353200	-0.65384200	1.36266000
C	1.16727100	-1.22233700	-2.21056500
H	1.89914700	-0.41860200	-2.26943900
H	1.63533200	-2.15176500	-2.54551000
H	0.32570000	-0.99103900	-2.86687800
C	2.75832300	-0.43628100	0.12160900
C	3.16591400	0.78472900	0.68344000
C	3.71252600	-1.29957200	-0.44076700
C	4.50917400	1.15147500	0.64875100

H	2.42374100	1.44114100	1.12643200
C	5.05809300	-0.93786500	-0.44878100
H	3.41040600	-2.26170800	-0.84360100
C	5.45555600	0.29039100	0.08649700
H	4.81936800	2.10511100	1.06495000
H	5.79587000	-1.61419700	-0.86953600
H	6.50377900	0.57388200	0.06952700
Ru	-1.21115000	-0.19609700	1.80918500
O	-0.75524800	1.58184500	0.67557500
C	-1.30374500	1.80581800	-0.43040200
O	-1.96259200	0.97492900	-1.11987100
C	-1.21436300	3.25761800	-0.95212700
F	-2.07420400	4.00925800	-0.23490700
F	-1.53862200	3.34089500	-2.24055800
F	0.02243800	3.73840900	-0.77692400