Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Synthesis of Oxazolidinones: Rhodium-Catalyzed C-H Amination of N-Mesyloxycarbamates.

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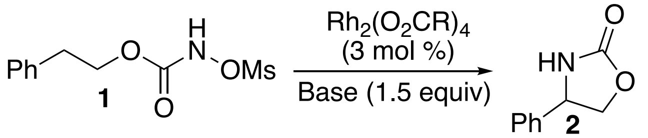
Supporting Information

Table of Contents

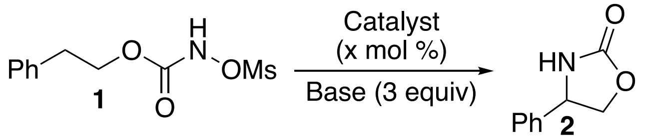
Table S1 - Screening of tetracarboxylate rhodium dimers as catalysts for the C-H amination of *N*-Mesyloxycarbamate 1



Entry	$Rh_2(O_2CR)_4$	Conditions[a]	Yield[b]
1	$Rh_2(OAc)_4$	K_2CO_3 aq. sat. MeOH, rt 16 h	16%
2	$Rh_2(OAc)_4$	KOAc solid MeOH, rt 16 h	61%
3	$Rh_2(OAc)_4$	KOAc solid (3 equiv) MeOH, rt 6 h	65%
4	$Rh_2(OAc)_4$	KOAc solid (3 equiv) EtOH, rt 16 h	36%
5	$Rh_2(oct)_4$	K_2CO_3 aq. sat. MeOH, rt 2 h	35%
6	$Rh_2(oct)_4$	KOAc solid (3 equiv) MeOH, rt 6 h	63%
7	$Rh_2(i\text{-val})_4$	K_2CO_3 solid (3 equiv) EtOAc, rt 2.5 h	26%
8	$Rh_2(i\text{-val})_4$	K_2CO_3 aq. sat. DCM, rt 3 h	26%
9	$Rh_2(esp)_2$	K_2CO_3 aq. sat. DCM, rt 16 h	45%
10	$Rh_2(esp)_2$	KOAc solid (3 equiv) MeOH, rt 6 h	65%
11	$Rh_2(tfa)_4$	KOAc solid (3 equiv) MeOH, rt 16 h	25%
12	$Rh_2(tfa)_4$	K_2CO_3 aq. sat. DCM, rt 16 h	7%

[a] 0.1M. [b] Isolated yields.

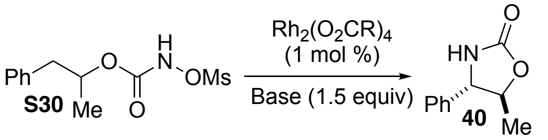
Table S2 - Screening of various organometallic species as catalysts for the C-H amination of *N*-Mesyloxycarbamate 1



Entry	Catalyst	Conditions[a]	Yield[b]
1	$FeBr_2$ (10 mol %)	K_2CO_3 solid DCM, rt 18 h	0%
2	Fe(TPP)Cl (10 mol %)	K_2CO_3 solid DCM, rt 18 h	0%
3	FePcCl (10 mol %)	K_2CO_3 solid $AgBF_4$ (10 mol %) DCM, rt 18 h	44%
4	FePcCl (10 mol %)	K_2CO_3 solid $AgBF_4$ (10 mol %) $Cl_2CHCHCl_2$, rt 18 h	63%
5	$Cu(OTf)_2$ (10 mol %)	KOAc solid DCM, rt 16 h, 4 Å MS	0%
6	$Cu(OTf)_2$ (10 mol %)	KOAc solid Terpyridine (30 mol %) DCM, rt 16 h, 4 Å MS	0%
7	AgOTf (10 mol %)	K_2CO_3 solid DCM, rt 16 h	0%
8	AgOTf (10 mol %)	K_2CO_3 solid Phenanthroline (30 mol %) DCM, rt 16 h	15%
9	AgOTf (10 mol %)	KOAc solid Terpyridine (30 mol %) DCM, rt 16 h, 4 Å MS	25%

[a] 0.1M. [b] Isolated yields.

Table S3 - Screening of of tetracarboxylate rhodium dimers as catalysts for the C-H amination of acyclic secondary *N*-Mesyloxycarbamate S30

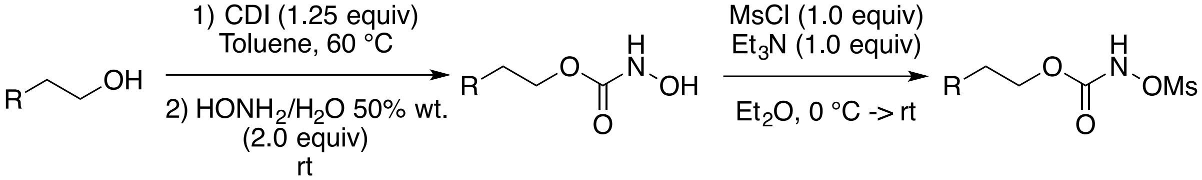


Entry	$Rh_2(O_2CR)_4$	Conditions[a]	Yield (dr)
1	$Rh_2(OAc)_4$	K_2CO_3 aq. sat. MeOH, rt 4 h	69% (89:11)
2	$Rh_2(OAc)_4$	K_2CO_3 solid MeOH, rt 4 h	31% (87:13)
3	$Rh_2(OAc)_4$	KOAc solid MeOH, rt 4 h	46% (90:10)
4	**$Rh_2(OAc)_4$**	**KOAc solid (3 equiv) MeOH, rt 4 h**	**79% (88:12)**
5	$Rh_2(OAc)_4$ 2 mol %	KOAc solid (3 equiv) MeOH, rt 2.5 h	73% (90:10)
6	$Rh_2(OAc)_4$	KOAc solid (3 equiv) MeOH (0.2 M), rt 3 h	66% (91:9)
7	$Rh_2(oct)_4$	K_2CO_3 aq. sat. MeOH, rt 4 h	9% (nd)
8	$Rh_2(oct)_4$	K_2CO_3 solid MeOH, rt 16 h	37% (82:18)
9	$Rh_2(oct)_4$	KOAc solid MeOH, rt 4 h	73% (88:12)
10	$Rh_2(oct)_4$	KOAc solid (3 equiv) MeOH, rt 5 h	70% (88:12)
11	**$Rh_2(oct)_4$ 2 mol %**	**KOAc solid (3 equiv) MeOH (0.2 M), rt 3 h**	**76% (89:11)**
12	$Rh_2(i\text{-val})_4$	K_2CO_3 aq. sat. DCM, rt 16 h	6% (81:19)
13	$Rh_2(esp)_2$ (3 mol%)	K_2CO_3 aq. sat. DCM, rt 16 h	33% (74:26)
14	$Rh_2(tpa)_4$ 3 mol %	K_2CO_3 aq. sat. DCM, rt 16 h	56% (53:43)
15	$Rh_2(tpa)_4$ 3 mol %	K_2CO_3 solid DCM, rt 16 h	68% (51:49)
16	$Rh_2(tpa)_4$ 3 mol %	K_2CO_3 aq. sat. EtOAc, rt 16 h	50% (53:47)
17	$Rh_2(tpa)_4$ 1.5 mol %	K_2CO_3 aq. sat. EtOAc, rt 16 h	19% (55:45)
18	$Rh_2(tpa)_4$ 3 mol %	K_2CO_3 solid EtOAc, rt 16 h	32% (55:45)
19	$Rh_2(tpa)_4$ 3 mol %	KOAc solid EtOAc, rt 16 h	39% (57:43)
20	$Rh_2(tpa)_4$ 3 mol %	KOAc solid (3 equiv) EtOAc, rt 16 h	16% (55:45)

[a] 0.1M.

Synthesis of *N*-Mesyloxycarbamates: General Procedures

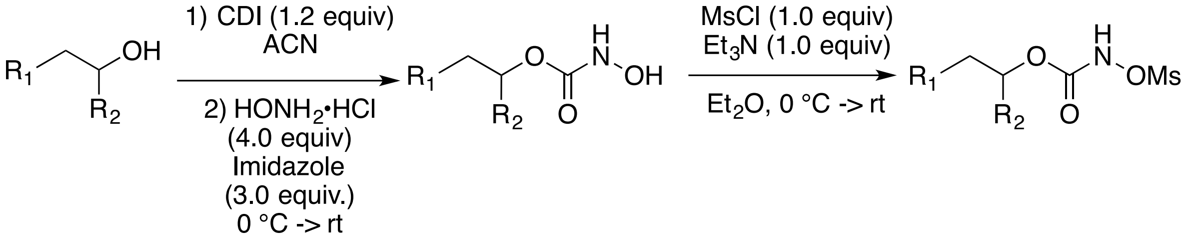
General procedure A



In a 250 mL round-bottom flask, equipped with a magnetic stir bar, carbonyl diimidazole (CDI) (2.03 g, 12.5 mmol, 1.25 equiv) was suspended in non-anhydrous toluene (100 mL). The suspension was heated to 60 °C and the alcohol (10.0 mmol, 1.00 equiv) was added. The homogeneous solution was stirred at 60 °C for 1 to 3 hours until complete disappearance of the starting alcohol. The reaction was monitored by TLC (EtOAc:Hexanes 4:6). The reaction mixture was allowed to cool to room temperature. Aqueous hydroxylamine solution 50% wt. (1.27 mL, 20.0 mL, 2.00 equiv) was added to the reaction mixture, which was vigorously stirred at room temperature until complete consumption of the intermediate, monitored by TLC (EtOAc:Hexanes 4:6). The reaction was quenched using a 1.2 N aqueous solution of HCl (60 mL). The layers were separated and the aqueous layer was extracted using EtOAc (3 x 60 mL). The combined organic layers were washed with brine, dried over sodium sulfate and filtered. The solvent was evaporated under reduced pressure yielding the desired *N*-hydroxycarbamate. For most substrates, the crude product was used without further purification in the next step. If needed, the crude product could be further purified by either a trituration in hexanes or a flash chromatography on silica gel eluting with EtOAc:Hexanes 4:6. All *N*-hydroxycarbamates were white solids.

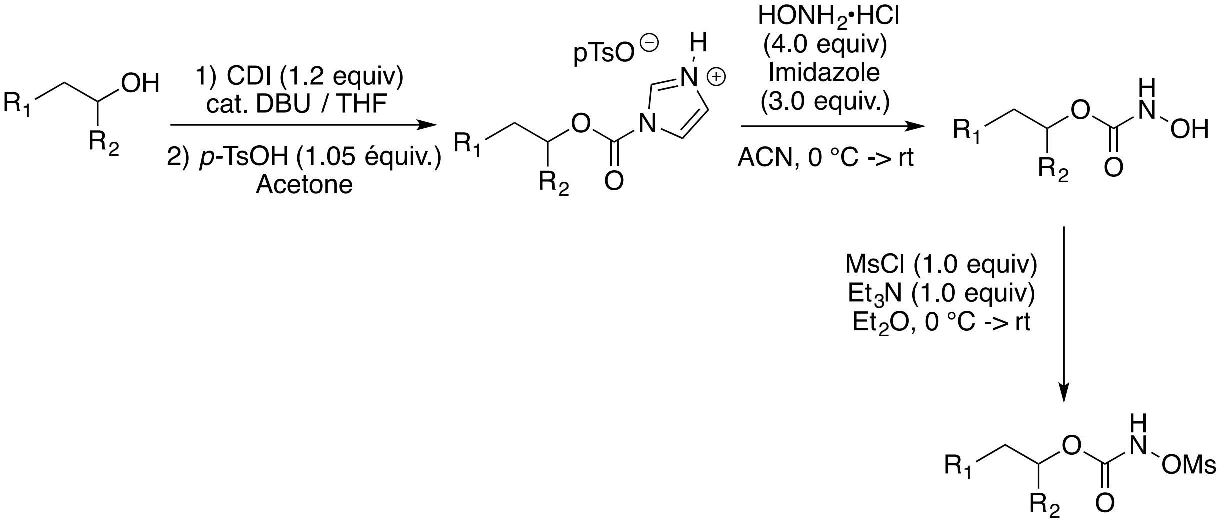
In a 250 mL, flame-dried round-bottom flask, equipped with a magnetic stir bar, under argon atmosphere, the *N*-hydroxycarbamate (1.00 equiv) was dissolved in anhydrous Et_2O (100 mL). At 0 °C, under argon, methanesulfonyl chloride (1.00 equiv, previously distilled under vaccum over P_2O_5) was added, followed by triethylamine (1.00 equiv, previously distilled over CaH_2). A white precipitate rapidly formed and the white suspension was stirred at room temperature, under argon, for 2 hours. The reaction was monitored by TLC (EtOAc:Hexanes 4:6). The reaction was quenched by addition of water (ca. 60 mL). The two layers were separated and the aqueous layer was extracted using Et_2O (3 x 60 mL). The combined organic layers were combined, washed with brine, dried over sodium sulfate and filtered. The solvent was removed under reduced pressure. The crude residue was chromatographed on silica gel eluting with EtOAc:Hexanes 25:75 to 30:70. Most of the synthesized *N*-mesyloxycarbamates were white solids.

General Procedure B



In a flame-dried 250 mL round-bottom flask, equipped with a magnetic stir bar, carbonyl diimidazole (CDI) (2.67 g, 16.5 mmol, 1.10 equiv) was dissolved in anhydrous MeCN (75 mL). The alcohol (15.0 mmol, 1.00 equiv) was then added and the mixture was stirred at room temperature for 2 hours. The reaction was monitored by TLC (EtOAc:Hexanes 4:6). The reaction mixture was cooled to 0 °C. Hydroxylamine hydrochloride (4.17 g, 60.0 mmol, 4.00 equiv) was added, followed by imidazole (3.06 g, 45.0 mmol, 3.00 equiv). Vigorous stirring was maintained for 1 hour at 0 °C then 1 hour at rt if needed until complete consumption of the intermediate. The mixture became homogeneous and a white precipitate appeared. The suspension was concentrated under vacuum and the residue was dissolved in 100 mL of a 1:1 (EtOAc:1.2 N HCl). The two layers were separated and the aqueous layer was extracted using EtOAc (2 x 80 mL). The combined organic layers were washed with brine, dried over Na_2SO_4 and filtered. The solvent the solvent was removed under reduced pressure yielding the desired *N*-hydroxycarbamate. If desired, the crude product could be further purified by flash chromatography on silica gel eluting with EtOAc:Hexanes 4:6 then 1:1. Most of the *N*-hydroxycarbamates were white solids. The mesylation of the *N*-hydroxycarbamate was performed as described in the **General procedure A**.

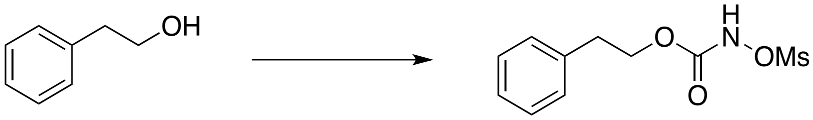
General Procedure C



In a flame-dried 250 mL round-bottom flask, equipped with a magnetic stir bar, carbonyl diimidazole (CDI) (1.78 g, 11.0 mmol, 1.10 equiv) was dissolved in anhydrous THF (57 mL). Under argon, the alcohol (10.0 mmol, 1.00 equiv) was added, followed by one drop of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU). The mixture was stirred at room temperature, under argon for 2 to 3 hours. The reaction was monitored by TLC (EtOAc:Hexanes 4:6). The solvent was evaporated under reduced pressure. Et_2O (25 mL) was added as well as water (25 mL). The two layers were separated. The organic layer was washed twice with water (2 x 25 mL), washed with brine, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure, yielding the desired intermediate. This intermediate was dissolved in acetone (40 mL) and *p*-toluenesulfonic acid (1.81 g, 10.5 mmol, 1.05 equiv) was added. The homogeneous mixture was stirred at rt for 30 minutes. The solvent was evaporated under reduced pressure. Diethyl ether (10 mL) was added and the solid was filtered out.

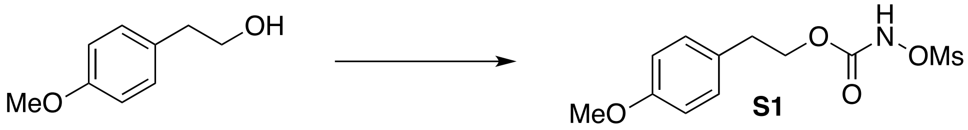
In a flame-dried 250 mL round-bottom flask, equipped with a magnetic stir bar, the *p*-toluenesulfonate salt (8 mmol, 1.00 equiv) was dissolved in anhydrous ACN (40 mL, 0.20 M). At 0 °C and under argon, hydroxylamine hydrochloride (2.24 g, 32.0 mmol, 4.00 equiv) and imidazole (1.63 g, 24.0 mmol, 3.00 equiv) were added and the reaction mixture was stirred at rt for 1 to 2 hours. The reaction was monitored by TLC (EtOAc:Hexanes 4:6). The solvent was evaporated under reduced pressure. Water was added (30 mL) followed by EtOAc (30 mL) and the two layers were separated. The aqueous layer was extracted with EtOAc (2 x 30 mL) and the combined organic layers were washed with brine, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure, yielding the desired *N*-hydroxycarbamate. If desired, the crude product could be further purified by flash chromatography on silica gel eluting with EtOAc:Hexanes 4:6 then 1:1. Most of the *N*-hydroxycarbamates were white solids. The mesylation of the *N*-hydroxycarbamate was performed as described in the **General procedure A**.

Characterization of *N*-Mesyloxycarbamates Derived from Primary Alcohols



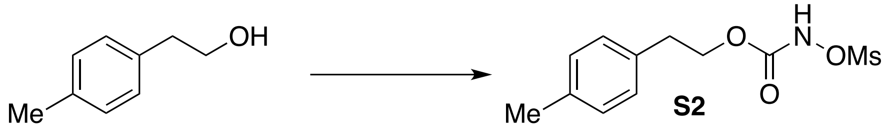
1

Phenethyl *N*-mesyloxycarbamate (1). The title compound was prepared according to general procedure A starting from phenethyl alcohol (12.2 g, 100.0 mmol). The *N*-hydroxycarbamate was isolated as a white solid (16.2 g, 89.4 mmol, 89% yield) after a trituration in hexanes. The mesylation of the *N*-hydroxycarbamate (8.10 g, 44.7 mmol) afforded **1** as a white solid (9.75 g, 37.6 mmol, 84% yield), after a flash chromatography on silica gel eluting with 30% EtOAc/hexanes. R$_f$ 0.4 (40% EtOAc/hexanes); mp 71.0-72.0 °C; ^{1}H NMR (500 MHz, CDCl$_3$) δ 8.34 (s (br), 1H), 7.36-7.32 (m, 2H), 7.29-2.23 (m, 3H), 4.49 (t, *J* = 8.5 Hz, 2H,), 3.05 (s, 3H), 3.02 (t, *J* = 8.5 Hz, 2H,); ^{13}C NMR (100 MHz, CDCl$_3$) δ 155.8, 136.8, 128.9, 128.6, 126.9, 67.8, 36.1, 34.9; IR (neat) 3246, 1736, 1485, 1376, 1247, 1173, 708 cm^{-1}; HRMS (ESI) calc. for $C_{10}H_{13}NNaO_5S$ [M+Na]$^+$: 282.0407; found: 282.0406.

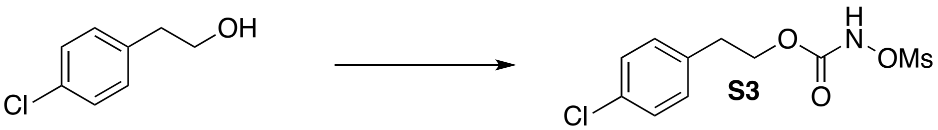


S1

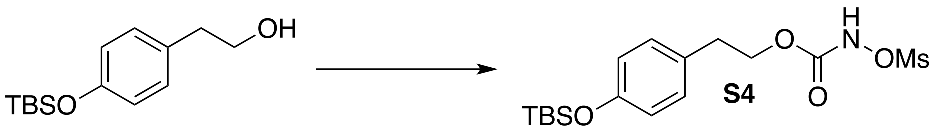
4-Methoxyphenethyl *N*-mesyloxycarbamate (S1). The title compound was prepared according to general procedure A starting from 2-(4-methoxyphenyl)ethanol (2.69 g, 17.7 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (3.59 g, 17.0 mmol, 96% yield). The mesylation of the *N*-hydroxycarbamate (1.67 g, 7.9 mmol) afforded **S1** as a white solid (1.73 g, 6.00 mmol, 76% yield) after a flash chromatography on silica gel eluting with 20% EtOAc/hexanes. R$_f$ 0.41 (40% EtOAc/hexanes); mp 60.8 °C; ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.38 (s (br), 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.85 (d, *J* = 8.0 Hz, , 2H), 4.41 (t, *J* = 8.0 Hz, 2H), 3.79 (s, 3H), 3.05 (s, 3H), 2.93 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 158.6, 156.0, 130.0, 129.0, 114.2, 68.0, 55.4, 36.2, 34.2; IR (neat) 3206, 1734, 1370, 1247, 816 cm^{-1}; HRMS (ESI) calc. for $C_{11}H_{15}NNaO_6S$ [M+Na]$^+$: 312.0512; found: 312.0523.



4-Methylphenethyl *N*-mesyloxycarbamate (*S*2). The title compound was prepared according to general procedure A starting from 2-(4-methylphenyl) ethanol (2.04 g, 15.0 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (2.36 g, 12.1 mmol, 81% yield). The mesylation of the *N*-hydroxycarbamate (1.17 g, 6.00 mmol) afforded **S2** as a white solid (1.49 g, 5.46 mmol, 91% yield) after a flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R_f 0.32 (30% EtOAc/hexanes); mp 69.9-61.7 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (s (br), 1H), 7.13-7.09 (m, 4H), 4.45 (t, *J* = 6.9 Hz, 2H), 3.05 (s, 3H), 2.96 (t, *J* = 7.5 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 136.5, 133.6, 129.4, 128.7, 67.9, 36.2, 34.6, 21.0; IR (neat) 3180, 1730, 1495, 1371, 1175, 1100, 809, 495 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{11}H_{15}NNaO_5S$ 296.0563; found 296.0571.



4-Chlorophenethyl *N*-mesyloxycarbamate (*S*3). The title compound was prepared according to general procedure A starting from 2-(4-chlorophenyl)ethanol (1.57 g, 10.0 mmol). The crude *N*-hydroxycarbamate was isolated as an impure beige solid (2.02 g, traces of starting alcohol by ^{1}H NMR). The mesylation of the crude *N*-hydroxycarbamate afforded **S3** as a white solid (1.51 g, 5.14 mmol, 51% yield over 2 steps) after a flash chromatography on silica gel eluting with 30% EtOAc/hexanes. R_f 0.45 (40% EtOAc/hexanes); mp 73.1-75.1 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (s (br), 1H), 7.31-7.28 (m, 2H), 7.16-7.14 (m, 2H), 4.41 (t, *J* = 7.0 Hz, 2H), 3.08 (s, 3H), 2.97 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 135.2, 132.8, 130.2, 128.8, 67.4, 36.2, 34.4; IR (neat) 3181, 1731, 1371, 1175, 806 cm^{-1}; HRMS (ESI) calc. For $C_{10}H_{12}ClNNaO_5S$ $[M+Na]^+$: 316.0017; found: 316.0028.



4-((*tert*-Butyldimethylsilyl)oxy)phenethyl *N*-mesyloxycarbamate (*S*4). The title compound was prepared according to general procedure A starting from 2-(4-((*tert*-butyldimethylsilyl)oxy)phenyl)ethan-1-ol[1] (2.55 g, 10.0 mmol). The *N*-hydroxycarbamate was isolated as a white solid (1.87 g) after a flash chromatography on silica gel eluting with EtOAc:Hexanes 4:6. The mesylation of the crude *N*-hydroxycarbamate afforded **S4** as pale yellow oil (1.52 g, 3.91 mmol, 39% yield over 2 steps) after a flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R_f 0.36 (30% EtOAc/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (s (br), 1H, N*H*), 7.07-7.04 (m, 2H), 6.79-6.76 (m, 2H), 4.42 (t, *J* = 7.0 Hz, 2H), 3.07 (s, 3H), 3.92 (t, *J* = 7.0 Hz, 2H), 0.98 (s, 9H), 0.19 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.7, 154.6, 129.8, 129.3, 120.2, 67.9, 36.2, 34.2, 25.6, 18.2, -4.45; IR (neat) 3279, 1743,

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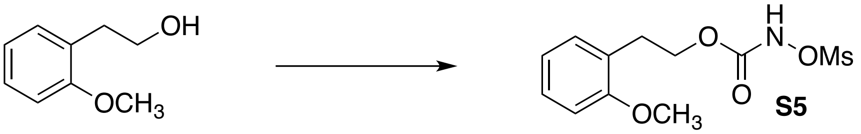
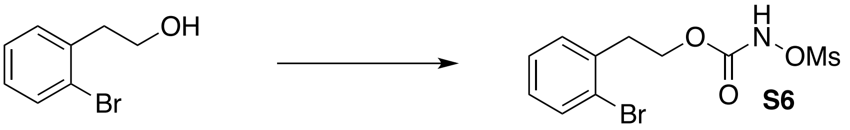
[1] S. N. Georgiades and J. Clardy, *Bioorg. Med. Chem. Lett.*, 2008, **18**, 3117.

1510, 1372, 1250, 1181 cm^{-1}; HRMS (APCI) calc. for $C_{16}H_{31}N_2O_6SSi$ $[M+NH_4]^+$: 407.1667; found: 407.1682.



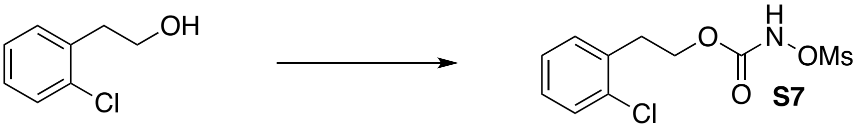
S5

2-Methoxyphenethyl *N*-mesyloxycarbamate (S5). The title compound was prepared according to general procedure A starting from 2-(2-methoxyphenyl) ethanol (1.89 g, 12.4 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (2.44 g, 11.6 mmol, 93% yield). The mesylation of the *N*-hydroxycarbamate (2.44 g, 11.5 mmol) afforded **S5** as a white solid (2.75 g, 9.50 mmol, 80% yield) after a flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R_f 0.33 (30% EtOAc/hexanes); mp 95.6-96.7 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (s (br), 1H), 7.24 (td, *J* = 8.1, 1.7 Hz, 1H), 7,13 (dd, *J* = 7.4, 1.6 Hz, 1H), 6.90 (td, *J* = 8.2 Hz, 1.05 Hz, 1H), 6.87 (d, *J* = 8.2 Hz, 1H), 4.46 (t, *J* = 6.8 Hz, 2H), 3.84 (s, 3H), 3.05 (s, 3H), 3.01 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.6, 155.7, 130.9, 128.3, 125.0, 120.5, 110.4, 66.8, 55.3, 36.2, 30.1; IR (neat) 3217, 1737, 1492, 1368, 1243, 1175, 1028, 754 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{11}H_{15}NNaO_6S$ 312.0512; found 312.0524.



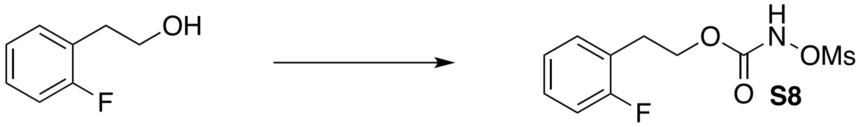
S6

2-Bromophenethyl *N*-mesyloxycarbamate (S6). The title compound was prepared according to general procedure A starting from 2-(2-bromophenyl) ethanol (1.56 g, 7.76 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (1.91 g, 7.37 mmol, 95% yield). The mesylation of the *N*-hydroxycarbamate (1.64 g, 6.32 mmol) afforded **S6** as a white solid (1.67 g, 4.94 mmol, 78% yield) after a flash chromatography on silica gel eluting with 20% EtOAc/hexanes. R_f 0.54 (30% EtOAc/hexanes 3:7); mp 86.4-87.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (s (br), 1H), 7.57 (dd, *J* = 8.0, 1 Hz, 1H) 7.29-7.24 (m, 2H), 7.15-7.11 (m, 1H), 4.49 (t, *J* = 6.8 Hz, 2H), 3.16 (t, *J* = 6.8 Hz, 2H), 3.10 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 136.2, 133.1, 131.2, 128.7, 127.6, 124.6, 66.2, 36.3, 35.3; IR (neat) 3277, 1748, 1472, 1375, 1239, 1172, 1086, 753 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{10}H_{12}BrNNaO_5S$ 359.9512; found 359.9509.



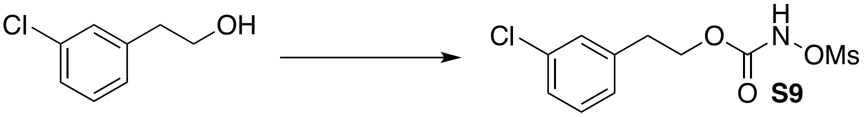
S7

2-Chlorophenethyl *N*-mesyloxycarbamate (S7). The title compound was prepared according to general procedure A starting from 2-(2-chlorophenyl) ethanol (2.00 g, 12.8 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (2.67 g, 12.4 mmol, 97% yield). The mesylation of the *N*-hydroxycarbamate (1.52 g, 6.95 mmol) afforded **S7** as a white solid (1.53 g, 5.21 mmol, 75% yield) after a flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R_f 0.37 (30% EtOAc/hexanes); mp 85.6-86.9 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (s, (br) 1H), 7.39-7.37 (m, 1H) 7.25-7.19 (m, 3H), 4.50 (t, *J* = 6.8 Hz, 2H), 3.15 (t, *J* = 6.8 Hz, 2H), 3.09 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 134.5, 134.2, 131.2, 129.8, 128.5, 127.0, 66.2, 36.2, 32.8; IR (neat) 3276, 1747, 1475, 1374, 1239, 1173, 1087, 756 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{10}H_{12}ClNNaO_5S$ 316.0017; found 316.0021.



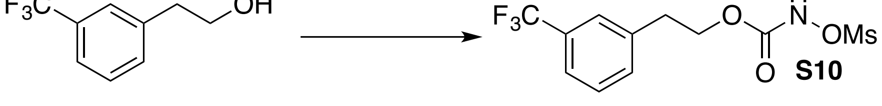
S8

2-Fluorophenethyl *N*-mesyloxycarbamate (S8). The title compound was prepared according to general procedure A starting from 2-(2-fluorophenyl) ethanol (1.88 g, 13.4 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (2.48 g, 12.5 mmol, 93% yield). The mesylation of the *N*-hydroxycarbamate (1.54 g, 7.53 mmol) afforded **S8** as a white solid (1.69 g, 6.10 mmol, 81% yield), after a flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R*f* 0.35 (30% EtOAc/hexanes); mp 78.8-79.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (s (br), 1H), 7.26-7.19 (m, 2H) 7.10 (td, *J* = 7.1, 1.1 Hz, 1H), 7.07-7.03 (m, 1H), 4.47 (t, *J* = 6.7 Hz, 2H), 3.09 (s, 3H), 3.05 (t, *J* = 6.6 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3 (d, *J* = 244 Hz), 155.5, 131.2 (d, *J* = 4.6 Hz), 128.9 (d, *J* = 8.2 Hz), 124.3 (d, *J* = 3.6 Hz), 123.8 (d, *J* = 16 Hz), 115.5 (d, *J* = 22 Hz), 66.7, 36.2, 28.7; ^{19}F NMR (471 MHz, $CDCl_3$) δ (ppm) -118.2; IR (neat) 3200, 1732, 1489, 1370, 1183, 1176, 809, 765 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{10}H_{12}FNNaO_5S$ 300.0312; found 300.0320.



S9

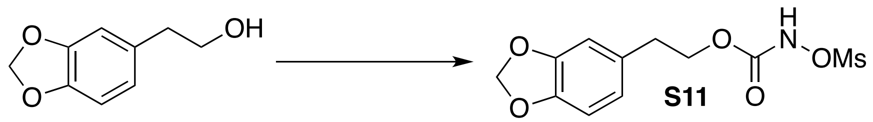
3-Chlorophenethyl *N*-mesyloxycarbamate (S9). The title compound was prepared according to general procedure A starting from 2-(3-chlorophenyl) ethanol (2.00 g, 12.8 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (2.53 g, 11.7 mmol, 92% yield). The mesylation of the *N*-hydroxycarbamate (1.36 g, 6.32 mmol) afforded **S9** as a white solid (1.57 g, 5.34 mmol, 84% yield), after a flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R*f* 0.55 (40% EtOAc/hexanes); mp 83.9-84.4 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (s (br), 1H), 7.27-7.21 (m, 3H) 7.11-7.09 (m, 1H), 4.46 (t, *J* = 6.8 Hz, 2H), 3.09 (s, 3H), 2.98 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 138.8, 134.4, 130.0, 129.0, 127.2, 127.1, 67.3, 36.3, 34.7; IR (neat) 3193, 1738, 1496, 1372, 1255, 1176, 966, 782 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{10}H_{12}ClNNaO_5S$ 316.0017; found 316.0005.



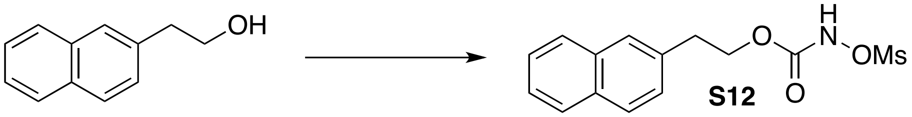
S10

3-(Trifluoromethyl)phenethyl *N*-mesyloxycarbamate (S10). The title compound was prepared according to general procedure A starting from 2-(3-(trifluoromethyl)phenyl) ethanol (2.50 g, 13.2 mmol. The crude *N*-hydroxycarbamate was isolated as a white solid (3.03 g, 12.2 mmol, 92% yield). The mesylation of the *N*-hydroxycarbamate (1.57 g, 6.33 mmol) afforded **S10** as a white solid (1.41 g, 4.31 mmol, 68% yield), after a flash chromatography on silica gel eluting with 20% EtOAc/hexanes. R*f* 0.5 (40%

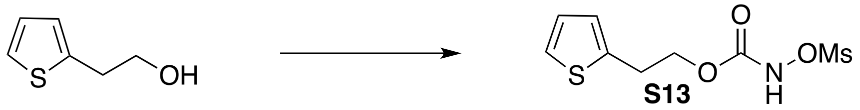
EtOAc/hexanes); mp 56.5-57.8 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (s (br), 1H), 7.54-7.52 (m, 1H), 7.47-7.41 (m, 3H), 4.49 (t, *J* = 6.8 Hz, 2H), 3.08 (s, 3H), 3.07 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.8, 137.8, 132,3, 130.9(q, *J* = 32 Hz), 129.1, 125.5 (q, *J* = 4 Hz), 124,0 (q, *J* = 271 Hz), 123.8 (q, *J* = 4 Hz), 67.1, 36.1, 34.7; ^{19}F NMR (471 MHz, $CDCl_3$) δ (ppm) -62.6; IR (neat) 3202, 1740, 1496, 1324, 1255, 1167, 1095, 793 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{11}H_{12}F_3NNaO_5S$ 350.0281; found 350.0289.



3,4-(Methylenedioxy)phenethyl *N*-mesyloxycarbamate (S11). The title compound was prepared according to general procedure A starting from 2-(3,4-(methylenedioxy)phenyl) ethanol (1.80 g, 10.8 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (2.30 g, 10.2 mmol, 94% yield). The mesylation of the *N*-hydroxycarbamate (1.42 g, 6.32 mmol) afforded **S11** as a white solid (1.44 g, 4.74 mmol, 75% yield) after a flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R_f 0.24 (30% EtOAc/hexanes); mp 111.9-112.4 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.0 (s (br), 1H), 6.75 (d, *J* = 7.9 Hz, 1H), 6,70 (d, *J* = 1.5 Hz, 1H), 6.66 (dd, *J* = 7.9, 1.5 Hz, 1H), 5.94 (s, 2H), 4.41 (t, *J* = 6.9 Hz, 2H), 3.11 (s, 3H), 2.91 (t, *J* = 6.9 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 147.8, 146.5, 130.4, 121.9, 109.2, 108.4, 101.0, 67.9, 36.3, 34.7; IR (neat) 3266, 1773, 1502, 1358, 1240, 1173, 1029, 528 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+NH_4]^+$ calcd for $C_{11}H_{17}N_2O_7S$ 321.0751; found 321.0753.

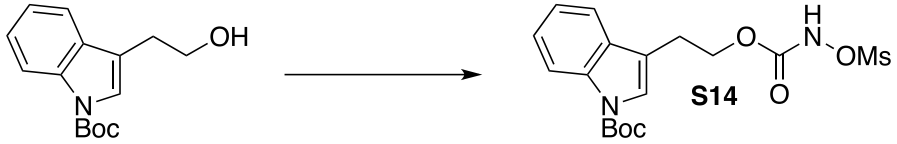


2-(Naphtalen-2-yl)ethyl *N*-mesyloxycarbamate (S12). The title compound was prepared according to general procedure A starting from 2-(naphtalen-2-yl)ethanol (3.15 g, 18.3 mmol). The *N*-hydroxycarbamate was isolated as a white solid (3.37 g, 14.6 mmol, 80% yield) after a flash chromatography on silica gel eluting with 40% EtOAc/hexanes. The mesylation of the *N*-hydroxycarbamate (3.13 g, 13.5 mmol) afforded **S12** as a white solid (3.50 g, 11.3 mmol, 84% yield), after a flash chromatography on silica gel eluting with 23% EtOAc/hexanes. R_f 0.38 (40% EtOAc/hexanes); mp 86.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s (br), 1H), 7.83-7.78 (m, 3H), 7.66 (s (br), 1H), 7.51-7.44 (m, 2H), 7.34 (dd, *J* = 8.4, 1.8 Hz, 1H), 4.55 (t, *J* = 8.0 Hz, 2H), 3.16 (t, *J* = 8.0 Hz, 2H), 2.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 134.2, 133.4, 132.3, 128.4, 127.6, 127.49, 127.47, 127.0, 126.3, 125.8, 67.6, 36.0, 35.2; IR (neat) 3328, 3227, 1740, 1367, 1243, 1173, 815 cm^{-1}; HRMS (ESI) calc. for $C_{14}H_{15}NNaO_5S$ $[M+Na]^+$: 332.0563; found: 332.0565.

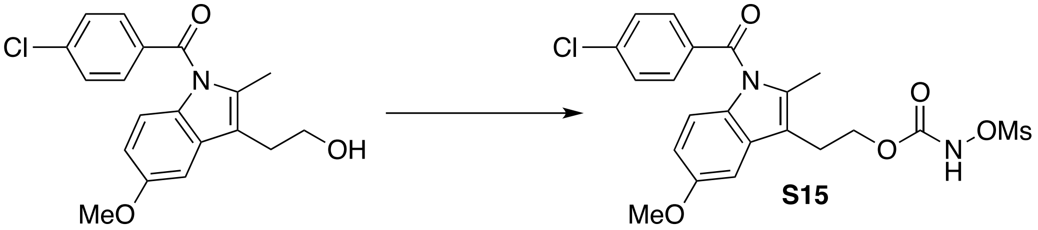


2-(Thiophen-2-yl)ethyl *N*-mesyloxycarbamate (S13). The title compound was prepared according to general procedure A starting from 2-thiopheneethanol (1.28 g, 10.0 mmol). The crude *N*-hydroxycarbamate was isolated a pale yellow solid (1.83 g, 9.80 mmol, 98%

yield). The mesylation of the *N*-hydroxycarbamate (1.83 g, 9.80 mmol) afforded **S13** as a white solid (2.04 g, 7.69 mmol, 77% yield over 2 steps) after a flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R_f 0.54 (40% EtOAc/hexanes); mp 33.0 °C; ^{1}H NMR (500 MHz, CDCl$_3$) δ 8.41 (s (br), 1H), 7.17 (dd, *J* = 5.0, 1.0 Hz, 1H), 6.95 (dd, *J* = 5.0, 3.5 Hz, 1H), 6.88-6.87 (m, 1H), 4.46 (t, *J* = 6.5 Hz, 2H), 3.22 (t, *J* = 6.5 Hz, 2H), 3.08 (s, 3H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 155.7, 138.8, 127.0, 125.9, 124.3, 67.4, 36.1, 29.2; IR (neat) 3236, 1734, 1374, 1175, 698 cm^{-1}; HRMS (ESI) calc. for $C_8H_{15}N_2O_5S_2$ [M+NH$_4$]$^+$: 283.0417; found: 283.0425.



***tert*-Butyl 3-(2-(((mesyloxy)carbamoyl)oxy)ethyl)-1*H*-indole-1-carboxylate (S14).** The title compound was prepared according to general procedure A starting from *tert*-butyl 3-(2-hydroxyethyl)-1*H*-indole-1-carboxylate[2] (13.92 g, 15.0 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid. The mesylation of the *N*-hydroxycarbamate afforded **S14** as a wax (23.6 g, 9.14 mmol, 61% yield over 2 steps) after a flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R_f 0.36 (40% EtOAc/hexanes); ^{1}H NMR (500 MHz, CDCl$_3$) δ 8.78 (s, 1H), 8.14 (s (br), 1H), 7.55 (d, *J* = 7.5 Hz), 7.50 (s (br), 1H), 7.37-7.34 (m, 1H), 7.30-7.27 (m, 1H), 4.53 (t, *J* = 6.8 Hz, 2H), 3.10 (t, *J* = 6.8 Hz, 2H), 3.09 (s, 3H), 1.70 (s, 9H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 156.0, 149.7, 135.2, 130.1, 124.5, 123.5, 122.6, 118.6, 115.8, 115.2, 83.9, 66.4, 36.0, 28.1, 24.4; IR (neat) 3400, 3270, 1749, 1380, 1174, 766 cm^{-1}; HRMS (ESI) calc. for $C_{17}H_{26}N_3NaO_7S$ [M+NH$_4$]$^+$: 421.1040; found: 421.1051.



2-(1-(4-Chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)ethyl *N*-mesyloxycarbamate (S15). The title compound was prepared according to general Procedure C starting from (4-chlorophenyl)(3-(2-hydroxyethyl)-5-methoxy-2-methyl-1*H*-indol-1-yl)methanone[3] (1.72 g, 5.00 mmol). The crude *p*-toluenesulfonate salt was isolated as a green solid (2.83 g, 4.64 mmol, 93% yield). The *p*-toluenesulfonate salt (2.75 g, 4.50 mmol) was reacted with hydroxylamine to produce the *N*-hydroxycarbamate as a bright yellow solid (0.869 g, 2.16 mmol, 48% yield) after a flash chromatography on silica gel eluting with 40% then 50% EtOAc/hexanes. The mesylation of the *N*-hydroxycarbamate (0.825 g, 2.05 mmol) afforded **S15** as pale yellow solid (0.297 g, 0.618 mmol, 30% yield) after a flash chromatography on silica gel eluting with 30%, then 50% EtOAc/hexanes. R_f 0.26 (40% EtOAc/hexanes); mp

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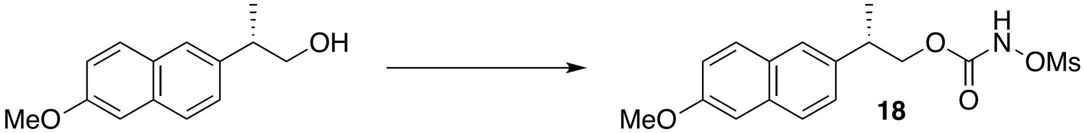
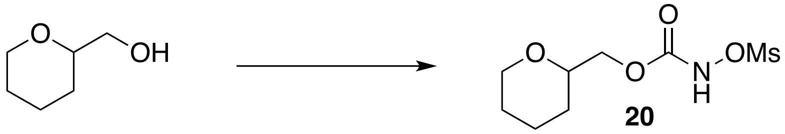
[2] N. Ghosh, S. Nayak and A. K. Sahoo, *J. Org. Chem.*, 2011, **76**, 500.

[3] S.-J. Wey, M. E. Augustyniak, E. D. Cochran, J. L. Ellis, X. Fang, D. S. Garvey, D. R. Janero, L. G. Letts, A. M. Martino, T. L. Melim, M. G. Murty, S. K. Richardson, J. D. Schroeder, W. M. Selig, A. M. Trocha, R. S. Wexler, D. V. Young, I. S. Zemtseva and B. M. Zifcak, *J. Med. Chem.*, 2007, **50**, 6367.

64-66 °C; ^{1}H NMR (500 MHz, CDCl$_3$) δ 8.08 (s (br), 1H), 7.66-7.64 (m, 2H), 7.49-7.46 (m, 2H), 6.93 (d, *J* = 2.5 Hz, 1H), 6.88 (d, *J* = 9.0 Hz, 1H), 6.68 (dd, *J* = 9.0, 2.5 Hz, 1H), 4.44 (t, *J* = 7.0 Hz, 2H), 3.85 (s, 3H), 3.08 (s, 3H), 3.07 (t, *J* = 7.0 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 168.3, 156.1, 155.7, 139.4, 135.6, 133.8, 131.1, 130.9 130.6, 129.2, 115.1, 114.2, 111.4, 101.0, 66.3, 55.8, 36.3, 23.7, 13.2; IR (neat) 2980, 1675, 1369, 1319, 1179, 1033 cm^{-1}; HRMS (ESI) calc. for $C_{21}H_{21}ClN_2NaO_7S$ [M+Na]$^+$: 503.0650; found: 503.0660.



(*S*)-2-(6-Methoxynaphthalen-2-yl)propyl *N*-mesyloxycarbamate (18). The title compound was prepared according to general procedure A starting from (*S*)-2-(6-methoxynaphthalen-2-yl)propan-1-ol[4] (99% *ee* purity) (2.52 g, 11.7 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid. The mesylation of the *N*-hydroxycarbamate afforded **18** as a white solid (0.852 g, 2.41 mmol, 21% yield over 2 steps) after a flash chromatography on silica gel eluting with 27% EtOAc/hexanes and a recrystallization in a CHCl$_3$/hexanes mixture. R_f 0.30 (40% EtOAc/hexanes); mp 104-106 °C; $[\alpha]_D^{20}$ = -26.1° (*c* 1.00, CHCl$_3$); ^{1}H NMR (500 MHz, CDCl$_3$) δ 8.19 (s (br), 1H), 7.70 (t, *J* = 7.5 Hz, 2H), 7.68 (s (br), 1H), 7.32 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.15 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.11-7.10 (m, 1H), 4.44-4.37 (m, 2H), 3.91 (s, 3H), 3.32-3.25 (m, 1H), 2.82 (s, 3H), 1.38 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 157.6, 155.8, 137.2, 133.6, 129.1, 128.9, 127.2, 125.9, 125.7, 119.1, 105.6, 71.9, 55.3, 38.9, 35.8, 17.8; IR (neat) 3235, 1749, 1709, 1410, 1178, 1021 cm^{-1}; HRMS (APCI) calc. for $C_{16}H_{23}N_2O_6S$ [M+NH$_4$]$^+$: 371.1271; found: 371.1263; Enantiomeric excess was determined by HPLC analysis : 98.5% *ee*, Chiracel® ADH, 1.00 mL/min, 95:5 hexanes/*i*-PrOH, 230 nm, t_R (minor) = 18.28 min, t_R (major) = 19.88 min.



(Tetrahydro-2*H*-pyran-2-yl)methyl *N*-mesyloxycarbamate (20). The title compound was prepared according to general procedure A starting from tetrahydropyran-2-methanol (3.48 g, 30.0 mmol). The mesylation of the *N*-hydroxycarbamate afforded **20** as a white solid (6.52 g, 25.8 mmol, 86% yield over 2 steps) after a flash chromatography on silica gel eluting with 47% EtOAc/hexanes. R_f 0.38 (50% EtOAc/hexanes); mp 75.8-77.4 °C; ^{1}H NMR (500 MHz, CDCl$_3$) δ 9.00 (s (br), 1H), 4.23 (dd, *J* = 11.5, 2.9 Hz, 1H), 4.13 (dd, *J* = 8.5, 7.4 Hz, 1H), 4.01-3.98 (m, 1H), 3.62-3.58 (m, 1H), 3.46-3.40 (m, 1H), 3.18 (s, 3H), 1.89-1.86 (m, 1H), 1.59-1.46 (m, 4H), 1.37-1.30 (m, 1H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 156.0, 75.2, 69.6, 68.3, 36.4, 27.2, 25.5, 22.7; IR (neat) 3397, 2850, 1752, 1364, 1168, 803 cm^{-1}; HRMS (ESI) calc. for $C_8H_{15}NNaO_6S$ [M+Na]$^+$: 276.0512; found: 276.0517.

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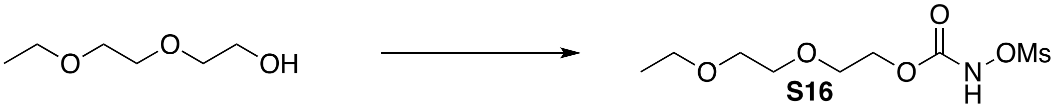
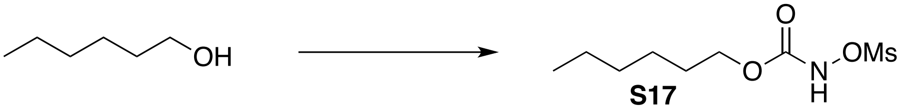
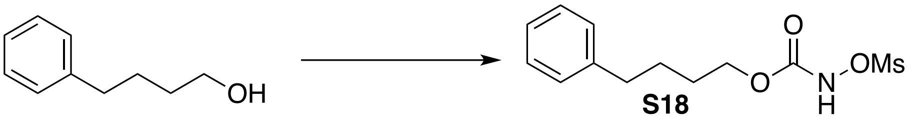
[4] E. Richmond, K. B. Ling, N. Duguet, L. B. Manton, N. Celebi-Olcum, Y.-H. Lam, S. Alsancak, A. M. Z. Slawin, K. N. Houk and A. D. Smith, *Org. Biomol. Chem.*, 2015, **13**, 1807.



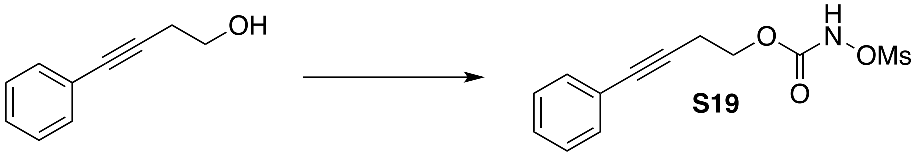
2-(2-Ethoxyethoxy)ethyl *N*-mesyloxycarbamate (S16). The title compound was prepared according to general procedure A (the aqueous hydroxylamine solution was added at 40 °C) starting from 2-(2-ethoxyethoxy)ethan-1-ol (1.34 g, 10.0 mmol). The mesylation of the *N*-hydroxycarbamate afforded **S16** as a white solid (0.36 g, 1.3 mmol, 14% yield over 2 steps) after a flash chromatography on silica gel eluting with 40%, then 60% EtOAc/hexanes. R_f 0.35 (60% EtOAc/hexanes); mp 40-42 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (s (br), 1H), 4.40-4.39 (m, 2H), 3.75-3.73 (m, 2H), 3.66-3.62 (m, 2H), 3.59-3.57 (m, 2H), 3.52 (q, *J* = 7.0 Hz, 2H), 3.20 (s, 3H), 1.21 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.8, 70.6, 69.7, 68.7, 66.7, 66.3, 36.4, 15.1; IR (neat) 3171, 2894, 1750, 1361, 1082 cm^{-1}; HRMS (ESI) calc. for $C_8H_{18}NO_7S$ $[M+H]^+$: 272.0799; found: 272.0807.



Hexyl *N*-mesyloxycarbamate (S17). The title compound was prepared according to general procedure A starting from hexan-1-ol (3.06 g, 30.0 mmol). The crude *N*-hydroxycarbamate was isolated as a colourless oil (4.14 g, 25.7 mmol, 86% yield) The mesylation of the *N*-hydroxycarbamate (4.03 g, 25.0 mmol) afforded **S17** as a white solid (4.99 g, 20.8 mmol, 83% yield) after a flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R_f 0.72 (40% EtOAc/Hexanes); mp 33.7-34.7 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (s (br), 1H), 4.23 (t, *J* = 7.0 Hz, 2H), 3.18 (s, 3H), 1.69-1.64 (m, 2H), 1.37-1.27 (m, 6H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.1, 67.8, 36.2, 31.2, 28.5, 25.2, 22.4, 13.9; IR (neat) 3166, 2933, 1720, 1367, 1179, 818 cm^{-1}; HRMS (ESI) calc. for $C_8H_{17}NNaO_5S$ $[M+Na]^+$: 262.0720; found: 262.0719.

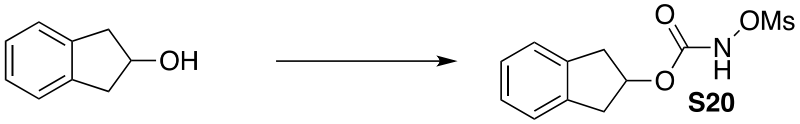


4-Phenylbutyl *N*-mesyloxycarbamate (S18). The title compound was prepared according to general procedure A starting from 4-phenylbutan-1-ol (1.50 g, 10.0 mmol). The mesylation of the *N*-hydroxycarbamate afforded **S18** as a white solid (1.77 g, 6.16 mmol, 62% yield over 2 steps) after a flash chromatography on silica gel eluting with 27% EtOAc/hexanes. R_f 0.61 (40% EtOAc/Hexanes); mp 82.1-83.7 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (s (br), 1H), 7.31-7.28 (m, 2H), 7.21-7.17 (m, 3H), 4.25 (t, *J* = 6.0 Hz, 2H), 3.15 (s, 3H), 2.65 (t, *J* = 7.0 Hz, 2H), 1.75-1.67 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.0, 141.6, 128.4, 128.3, 125.9, 67.5, 36.2, 35.2, 28.0, 27.3; IR (neat) 3210, 1733, 1370, 1181, 749 cm^{-1}; HRMS (ESI) calc. for $C_{12}H_{21}N_2O_5S$ $[M+NH_4]^+$: 305.1166; found: 305.1175.

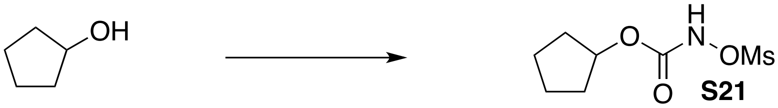


4-Phenylbut-3-yn-1-yl *N*-mesyloxycarbamate (S19). The title compound was prepared according to general procedure A starting from 4-phenylbut-3-yn-1-ol[5] (1.46 g, 10.0 mmol). The mesylation of the *N*-hydroxycarbamate afforded **S19** as a white solid (1.84 g, 6.50 mmol, 65% yield over 2 steps) after a flash chromatography on silica gel eluting with 27% EtOAc/hexanes. R_f 0.62 (40% EtOAc/Hexanes); mp 79.1-80.1 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (s (br), 1H), 7.40-7.38 (m, 2H), 7.31-7.28 (m, 3H), 4.42 (t, *J* = 6.5 Hz, 2H), 3.16 (s, 3H), 2.82 (t, *J* = 6.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 131.6, 128.3, 128.2, 122.8, 84.5, 82.5, 65.1, 36.3, 20.1; IR (neat) 3282, 1757, 1374, 1170, 972, 752 cm^{-1}; HRMS (ESI) calc. for $C_{12}H_{13}NNaO_5S$ [M+Na]$^+$: 306.0407; found: 306.0402.

Characterization of *N*-Mesyloxycarbamates Derived from Cyclic Secondary Alcohols



2,3-Dihydro-1*H*-inden-2-yl *N*-mesyloxycarbamate (S20). The title compound was prepared according to general procedure A (the aqueous hydroxylamine solution was added at 40 °C) starting from 2-indanol (4.03 g, 30.0 mmol). The crude *N*-hydroxycarbamate was isolated a beige solid (5.38 g, 27.8 mmol, 93% yield). The mesylation of the *N*-hydroxycarbamate (2.51 g, 13.0 mmol) afforded **S20** as a white solid (2.82 g, 10.4 mmol, 80% yield) after a flash chromatography on silica gel eluting with 23% EtOAc/hexanes. R_f 0.42 (40% EtOAc/Hexanes); mp 109.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s (br), 1H), 7.29-7.22 (m, 4H), 5.65-5.61 (m, 1H), 3.37 (dd, *J* = 17, 6.0 Hz, 2H), 3.12 (dd, *J* = 17, 2.0 Hz, 2H), 3.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 139.6, 127.1, 124.7, 79.3, 39.5, 36.3; IR (neat) 3287, 1731, 1367, 1467, 1182, 743, 710 cm^{-1}; HRMS (ESI) calc. for $C_{11}H_{13}NNaO_5S$ [M+Na]$^+$: 294.0407; found: 294.0412.



Cyclopentyl *N*-mesyloxycarbamate (S21). The title compound was prepared according to general procedure B starting from cylopentanol (1.92 ml, 21.0 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (2.79 g, 19.2 mmol, 96% yield). The mesylation of the *N*-hydroxycarbamate (2.00 g, 13.7 mmol) afforded **S21** (1.50 g, 6.72 mmol, 49% yield) as a white solid after flash chromatography on silica gel eluting with 20%, then 30% AcOEt/Hexanes. R_f 0.58 (40% EtOAc/Hexanes); mp 77.1-78.7 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (s (br), 1H), 5.27-5.24 (m, 1H), 3.18 (s, 3H), 1.93-1.86 (m, 2H), 1.81-1.69 (m, 4H),

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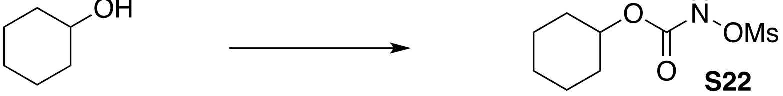
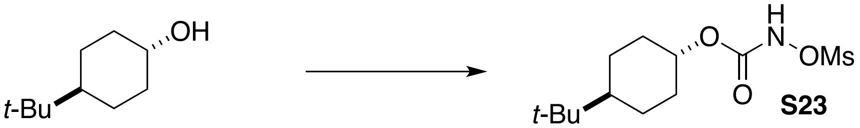
[5] J. Panteleev, R. Y. Huang, E. K. J. Lui and M. Lautens, *Org. Lett.*, 2011, **13**, 5314.

1.67-1.59 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 81.3, 36.3, 32.6, 23.5; IR (neat) 3202, 1725, 1373, 1267, 1178, 1096, 765, 492 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_7H_{13}NNaO_5S$ 246.0466; found 246.0399.



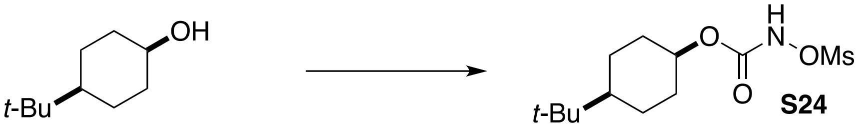
S22

Cyclohexyl *N*-mesyloxycarbamate (S22). The title compound was prepared according to general procedure A starting from cyclohexanol (2.09 g, 20.0 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (2.90 g, 18.2 mmol, 91% yield). The mesylation of the *N*-hydroxycarbamate (2.00 g, 12.5 mmol) afforded **S22** (2.14 g, 9.02 mmol, 72% yield) as a white solid after flash chromatography on silica gel eluting with 20%, then 30% AcOEt/Hexanes. R_f 0.76 (40% EtOAc/Hexanes); mp 81.7-82.4 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (s (br), 1H), 4.84-4.79 (m, 1H), 3.19 (s, 3H), 1.94-1.89 (m, 2H), 1.77-1.71 (m, 2H), 1.58-1.45 (m, 3H) 1.42-1.34 (m, 2H), 1.31-1.23 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 76.9, 36.2, 31.4, 25.0, 23.4; IR (neat) 3152, 2938, 1721, 1367, 1180, 1084, 771, 501 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_8H_{15}NNaO_5S$ 260.0563; found 260.0570.



S23

***trans*-4-(*tert*-Butyl)cyclohexyl *N*-mesyloxycarbamate (S23).** The title compound was prepared according to general procedure B starting from (±)-*trans*-4-(*tert*-butyl)cyclohexanol[6] (2.00 g, 12.8 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (2.50 g, 11.6 mmol, 91% yield). The mesylation of the *N*-hydroxycarbamate (0.53 g, 6.97 mmol) afforded **S23** (1.33 g, 4.53 mmol, 65% yield) as a white solid after flash chromatography on silica gel eluting with 20% AcOEt/Hexanes. R_f 0.75 (40% EtOAc/Hexanes); mp 90.4-91.8 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (s (br), 1H), 4.70-4.63 (m, 1H), 3.16 (s, 3H), 2.10-2.06 (m, 2H), 1.84-1.81 (m, 2H), 1.39-1.31 (m, 2H), 1.14-1.05 (m, 2H), 1.02-0.96 (m, 1H), 0.84 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 77.8, 46.8, 36.2, 32.2, 31.9, 27.5, 25.2; IR (neat) 3249, 2945, 2867, 1730, 1377, 1257, 1179, 1084, 788, 489 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{12}H_{23}NNaO_5S$ 316.1190; found 316.1202.



S24

***cis*-4-(*tert*-Butyl)cyclohexyl *N*-mesyloxycarbamate (S24).** The title compound was prepared according to general procedure B starting from (±)-*cis*-4-(*tert*-butyl)cyclohexanol[7] (2.00 g, 12.8 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (2.60 g, 12.8 mmol, 94% yield). The mesylation of the *N*-hydroxycarbamate (1.50 g, 6.97 mmol) afforded **S24** (1.37 g, 4.67 mmol, 67% yield) as a white solid after flash chromatography on silica gel eluting with 20% AcOEt/Hexanes. R_f 0.70 (40%

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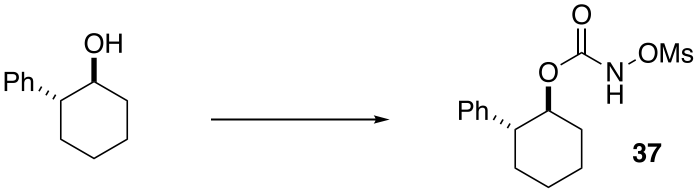
[6] E. L. Eliel, R. J. L. Martin and D. Nasipuri, *Org. Synth.*, 1967, **47**, 16.

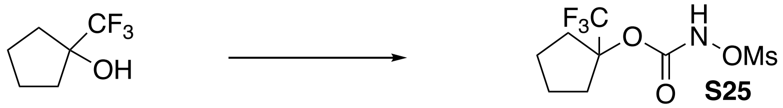
[7] H. C. Brown and S. Krishnamurthy, *J. Am. Chem. Soc.*, 1972, **94**, 7159.

EtOAc/Hexanes); mp 104.9-105.5 °C; ^{1}H NMR (500 MHz, CDCl$_3$) δ 8.05 (s (br), 1H), 5.10-5.08 (m, 1H), 3.20 (s, 3H), 2.05-2.00 (m, 2H), 1.64-1.61 (m, 2H), 1.56-1.50 (m, 2H), 1.28-1.20 (m, 2H), 1.07-1.01 (m, 1H), 0.86 (s, 9H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 155.5, 74.1, 47.3, 36.3, 32.5, 30.5, 27.4, 21.5; IR (neat) 3208, 2868, 1718, 1489, 1380, 1273, 1182, 770, 500 cm^{-1}; HRMS (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_{12}H_{23}NNaO_5S$ 316.1190; found 316.1201.

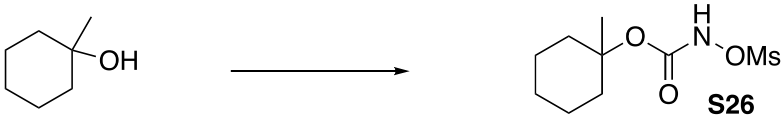


(±)-*trans*-2-Phenylcyclohexyl *N*-mesyloxycarbamate (37). The title compound was prepared according to general procedure A starting from (±)-*trans*-2-phenylcyclohexanol (2.12 g, 12.0 mmol). The crude *N*-hydroxycarbamate was isolated as a viscous oil (2.78 g, 11.8 mmol, 50% yield). The mesylation of the *N*-hydroxycarbamate (1.40 g, 5.97 mmol) afforded **32** (1.28 g, 4.09 mmol, 69% yield) as a white solid after flash chromatography on silica gel eluting with 30% AcOEt/Hexanes. R$_f$ 0.64 (40% EtOAc/Hexanes); mp 99.5.4-101.5 °C; ^{1}H NMR (500 MHz, CDCl$_3$) δ 7.74 (s (br), 1H), 7.30-7.27 (m, 2H), 7.21-7.18 (m, 3H), 5.07-5.01 (m, 1H), 2.73-2.67 (m, 1H), 2.68 (s, 3H), 2.23-2.20 (m, 1H), 1.98-1.89 (m, 2H), 1.82-1.77 (m, 1H) 1.60-1.45 (m, 3H), 1.41-1.32 (m, 1H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 155.0, 142.3, 128.6, 127.5, 126.8, 90.0, 49.9, 35.4, 34.0 32.2, 25.5, 24.7; IR (neat) 3297, 2940, 1736, 1445, 1364, 1247, 1179, 758, 701, 496 cm^{-1}; HRMS (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_{14}H_{19}NNaO_5S$ 336.0876; found 336.0880.

Characterization of *N*-Mesyloxycarbamates Derived from Cyclic Tertiary Alcohols

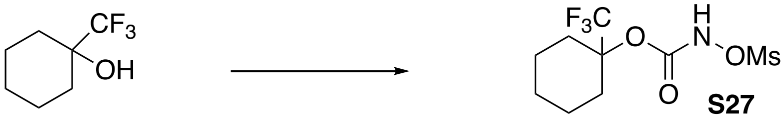


1-Trifluoromethyl-cyclopentyl *N*-mesyloxycarbamate (S25). The title compound was prepared according to general procedure C using 1-trifluoromethyl-cyclopentanol (1.00 g, 6.49 mmol, 1.00 equiv). The crude *N*-hydroxycarbamate was isolated as a white solid (0.81 g, 3.81 mmol, 87% yield). The mesylation of the *N*-hydroxycarbamate (0.58 g, 2.72 mmol) afforded **S25** (0.55 g, 1.90 mmol, 70% yield) as a white solid after flash chromatography on silica gel eluting with 20% AcOEt/Hexanes. R$_f$ 0.77 (40% EtOAc/Hexanes); mp 74.7-76.1 °C; ^{1}H NMR (500 MHz, CDCl$_3$) δ 8.18 (s (br), 1H), 3.18 (s, 3H), 2.35-2.29 (m, 2H), 2.22-2.16 (m, 2H), 2.06-1.98 (m, 2H), 1.77-1.70 (m, 2H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 152.9, 125.0 (q, J = 282 Hz), 92.0 (q, J = 30 Hz), 36.5, 33.0, 25.3; ^{19}F NMR (471 MHz, CDCl$_3$) δ (ppm) -80.0; IR (neat) 3314, 1772, 1443, 1327, 1160, 777, 767, 535, 520 cm^{-1}; HRMS (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_8H_{12}F_3NNaO_5S$ 314.0281; found 314.0270.



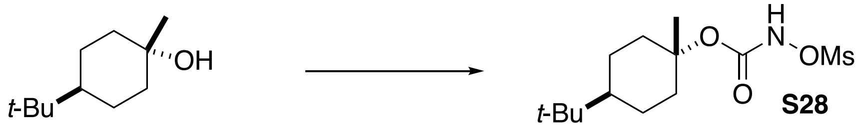
S26

1-Methylcyclohexyl *N*-mesyloxycarbamate (S26). The title compound was prepared according to general procedure C starting from 1-methylcyclohexanol (3.54 g, 31.0 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (0.65 g, 3.78 mmol, 72% yield). The mesylation of the *N*-hydroxycarbamate (0.57 g, 3.29 mmol) afforded **S26** (0.560 g, 2.24 mmol, 68% yield) as a white solid after flash chromatography on silica gel eluting with 20% AcOEt/Hexanes. R_f 0.44 (40% EtOAc/Hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 (s (br), 1H), 3.16 (s, 3H), 2.14-2.11 (m, 2H), 1.58-1.44 (m, 7H), 1.30-1.25 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.6, 86.3, 36.5, 36.2, 25.3, 25.0, 21.9; IR (neat) 3279, 2936, 2863, 1734, 1449, 1328, 1268, 1236, 1148, 1102, 1006, 868, 794, 704, 647, 482 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+K]^+$ calcd for $C_9H_{17}NKO_5S$ 290.0459; found 290.0468.



S27

1-Trifluoromethyl-cyclohexyl *N*-mesyloxycarbamate (S27). The title compound was prepared according to general procedure C starting from 1-trifluoromethyl-cyclohexanol (1.00 g, 5.97 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (0.66 g, 2.84 mmol, 80% yield). The mesylation of the *N*-hydroxycarbamate (0.58 g, 2.55 mmol) afforded **S27** (0.53 g, 1.74 mmol, 68% yield) as a white solid after flash chromatography on silica gel eluting with 20% AcOEt/Hexanes. R_f 0.65 (40% EtOAc/Hexanes); mp 87.9-88.6 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (s (br), 1H), 3.19 (s, 3H), 2.55-2.52 (m, 2H), 1.77-1.71 (m, 3H), 1.65-1.59 (m, 2H), 1.54-1.43 (m, 2H), 1.35-1.26 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.8, 124.5 (q, J = 285 Hz), 84.4 (q, J = 29 Hz), 36.5, 28.5, 24.3, 20.5; ^{19}F NMR (471 MHz, $CDCl_3$) δ (ppm) -79.7; IR (neat) 3314, 3042, 2942, 2870, 1774, 1451, 1439, 1240, 1164, 1071, 966, 761, 686, 539, 514 cm^{-1}; HRMS (ESI-TOF) m/z: $[M+NH_4]^+$ calcd for $C_9H_{18}F_3N_2O_5S$ 323.0883; found 323.0883.



S28

***trans*-4-(*tert*-Butyl)-1-methylcyclohexyl *N*-mesyloxycarbamate (S28).** The title compound was prepared according **to general procedure C** starting from (±)-*trans*-4-(*tert*-butyl)-1-methylcyclohexanol[8] (1.30 g, 7.63 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (1.51 g, 6.59 mmol, 96% yield). The mesylation of the *N*-hydroxy-carbamate (1.40 g, 6.01 mmol) afforded **S28** (1.22 g, 3.97 mmol, 65% yield) as a white solid after flash chromatography on silica gel eluting with 20% AcOEt/Hexanes. R_f 0.77 (40% EtOAc/Hexanes); mp 110.3-110.9 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (s (br), 1H), 3.17 (s, 3H), 2.20-2.17 (m, 2H), 1.77-1.61 (m, 4H), 1.56 (s, 3H), 1.16-1.04 (m, 3H), 0.85 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.4, 87.9, 47.3, 37.0, 36.4, 32.2, 27.5, 24.3, 21.6; IR (neat) 3311,

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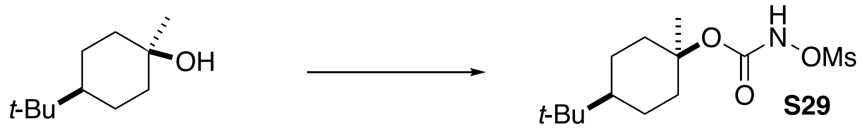
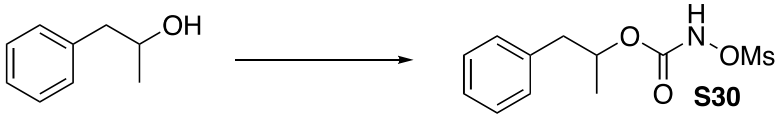
[8] W. J. Houlihan, *J. Org. Chem.*, 1962, **27**, 3860.

2946, 1762, 1364, 1246, 1188, 1107, 518 cm^{-1}; HRMS (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_{13}H_{25}NNaO_5S$ 330.1354; found 330.1347.

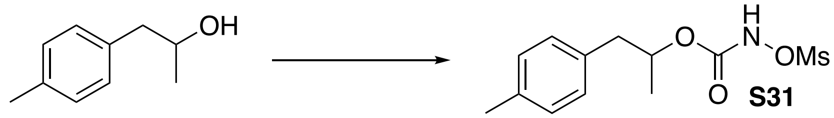

S29

***cis*-4-(*tert*-Butyl)-1-methylcyclohexyl *N*-mesyloxycarbamate (S29).** The title compound was prepared according to general procedure C starting from (±)-*cis*-4-(*tert*-butyl)-1-methylcyclohexanol[8] (1.50 g, 8.81 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (1.40 g, 6.11 mmol, 89% yield). The mesylation of the *N*-hydroxycarbamate (1.40 g, 6.10 mmol) afforded **S27** (1.16 g, 3.78 mmol, 62% yield) as a white solid after flash chromatography on silica gel eluting with 20% AcOEt/Hexanes. R$_f$ 0.78 (40% EtOAc/Hexanes); mp 101.3-102.1 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (s (br), 1H), 3.17 (s, 3H), 2.20-2.17 (m, 2H), 1.77-1.73 (m, 2H), 1.70-1.64 (m, 2H), 1.56 (s, 3H), 1.17-1.02 (m, 3H), 0.86 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.3, 87.9, 47.4, 37.1, 36.4, 32.2, 27.5, 24.3, 21.6; IR (neat) 3310, 2983, 2946, 1762, 1364, 1246, 1188, 1107, 518 cm^{-1}; HRMS (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_{13}H_{25}NNaO_5S$ 330.1351; found 330.1346.

Characterization of *N*-Mesyloxycarbamates Derived from Acyclic Secondary Alcohols


S30

(±)-1-Phenylpropan-2-yl *N*-mesyloxycarbamate (S30). The title compound was prepared according to general procedure C starting from 1-phenylpropan-2-ol (5.12 g, 37.5 mmol). *N*-Mesyloxycarbamate **S30** was obtained as a thick oil (6.48 g, 23.7 mmol, 63% yield over 2 steps) after flash chromatography on silica gel eluting with 20% EtOAc/Hexanes. R$_f$ 0.35 (30% EtOAc/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (s (br), 1H), 7.32-7.29 (m, 2H), 7.25-7.19 (m, 3H), 5.22-5.16 (m, 1H), 3.02 (s, 3H), 2.95 (dd, *J* = 14, 7.1 Hz, 1H), 2.85 (dd, *J* = 14, 6.1 Hz, 1H), 1.33 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.5, 136.7, 129.6, 128.7, 127.0, 75.7, 42.3, 36.2, 19.7; IR (neat) 3285, 3030, 2983, 2938, 1740, 1495, 1454, 1414, 1372, 1327, 1248, 1182, 1133, 1078, 1032, 970, 789, 749, 702 cm^{-1}; HMRS (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_{11}H_{15}NNaO_5S$ 296.0563; found 296.0570.


S31

(±)-1-*p*-Tolylpropan-2-yl *N*-methylsulfonyloxycarbamate (S31). The title compound was prepared according to general procedure C starting from 1-(p-tolyl)propan-2-ol[9] (2.61 g, 17.4 mmol). *N*-Mesyloxycarbamate **S31** was obtained as a thick oil (1.47 g, 5.11 mmol,

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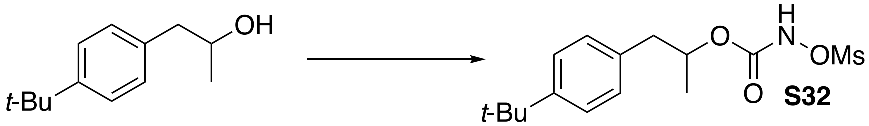
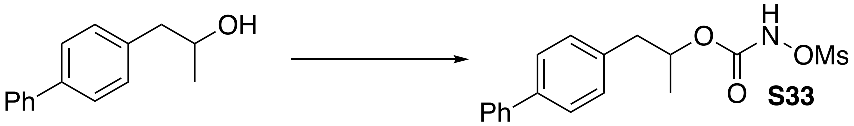
[9] X. Du, Y. Zhang, D. Peng and Z. Huang, *Angew. Chem., Int. Ed.*, 2016, **55**, 6671.

30% yield over 2 steps) after flash chromatography on silica gel eluting with 20% EtOAc/hexanes. R_f 0.38 (30% EtOAc/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (s (br), 1H), 7.12-7.07 (m, 4H), 5.20-5.13 (m, 1H), 3.04 (s, 3H), 2.92 (dd, *J* = 14, 7.1 Hz, 1H), 2.82 (dd, *J* = 14, 6.1 Hz, 1H), 2.32 (s, 3H), 1.31 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.5, 136.6, 133.6, 129.42, 129.36, 75.9, 41.9, 36.2, 21.2, 19.7; IR (neat) 3274, 3021, 2982, 2936, 2867, 1736, 1515, 1452, 1414, 1370, 1325, 1250, 1181, 1112, 1080, 1045, 969, 918, 803, 771, 711 cm^{-1}; HMRS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{12}H_{17}NNaO_5S$ 310.0720; found 310.0722.



S32

(±)-1-(4-(*tert*-Butyl)phenyl)propan-2-yl *N*-methylsulfonyloxycarbamate (S32). The title compound was prepared according to general procedure C starting from 1-(4-(*tert*-butyl)phenyl)propan-2-ol[10] (2.20 g, 11.4 mmol). *N*-Mesyloxycarbamate **S32** was obtained as a sticky oil (1.24 g, 3.76 mmol, 32% yield over 2 steps) after flash chromatography on silica gel eluting with 20% EtOAc/hexanes. R_f 0.47 (30% EtOAc/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (s (br), 1H), 7.32 (d, *J* = 8.3 Hz, 2H), 7.12 (d, *J* = 8.4 Hz, 2H), 5.22-5.15 (m, 1H), 3.01 (s, 3H), 2.93 (dd, *J* = 14, 7.1 Hz, 1H), 2.83 (dd, *J* = 14, 6.1 Hz, 1H), 1.33 (d, *J* = 6.3 Hz, 3H), 1.30 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.4, 149.9, 133.6, 129.2, 125.6, 75.9, 41.7, 36.3, 34.6, 31.5, 19.8; IR (neat) 3282, 3024, 2961, 2870, 1739, 1513, 1461, 1413, 1369, 1326, 1247, 1180, 1135, 1077, 1047, 1019, 969, 920, 830, 801, 771, 711 cm^{-1}; HMRS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{15}H_{23}NNaO_5S$ 352.1189; found 352.1197.



S33

(±)-1-(Biphenyl-4-yl)propan-2-yl *N*-methylsulfonyloxycarbamate (S33). The title compound was prepared according to the general procedure C starting from 1-([1,1'-biphenyl]-4-yl)propan-2-ol[11] (4.12 g, 19.4 mmol). *N*-Mesyloxycarbamate **S33** was obtained as an off-white solid (2.51 g, 7.18 mmol, 37% yield over 2 steps) after flash chromatography on silica gel eluting with 20% EtOAc/hexanes. R_f 0.30 (30% EtOAc/hexanes); mp 93-94 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (s (br), 1H), 7.58-7.56 (m, 2H), 7.56-7.53 (m, 2H), 7.46-7.41 (m, 2H), 7.37-7.27 (m, 3H), 5.28-5.20 (m, 1H), 3.00 (s, 3H), 2.99 (dd, *J* = 14, 6.9 Hz, 1H), 2.91 (dd, *J* = 14, 6.0 Hz, 1H), 1.37 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.4, 140.8, 140.0, 135.8, 130.0, 129.0, 127.5, 127.4, 127. 1, 75.7, 42.0, 36.3, 19.8; IR (neat) 3285, 3033, 2986, 2938, 2863, 1734, 1524, 1486, 1411, 1371, 1326, 1247, 1217, 1178, 1134, 1079, 1044, 1006, 965, 908, 858, 843, 760, 730, 708 cm^{-1}; HMRS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{17}H_{19}NNaO_5S$ 372.0876; found 372.0881.

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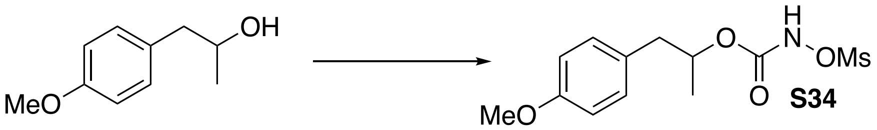
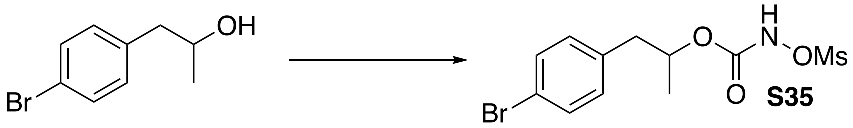
[10] Y. Zhao and D. J. Weix, *J. Am. Chem. Soc.*, 2014, **136**, 48.

[11] W. Zhang, F. Wang, S. D. McCann, D. Wang, P. Chen, S. S. Stahl and G. Liu, *Science*, 2016, **353**, 1014.



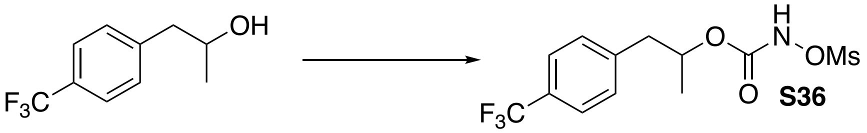
S34

(±)-1-(4-Methoxyphenyl)propan-2-yl *N*-methylsulfonyloxycarbamate (S34). The title compound was prepared according to general procedure C starting from 1-(4-methoxyphenyl)propan-2-ol[10] (2.59 g, 15.6 mmol). *N*-Mesyloxycarbamate **S34** was obtained as off-white crystals (2.37 g, 7.81 mmol, 50% yield over 2 steps) after flash chromatography on silica gel eluting with 20% EtOAc/hexanes. R$_f$ 0.26 (30% EtOAc/hexanes); mp 52-54 °C; ^{1}H NMR (500 MHz, CDCl$_3$) δ 7.96 (s (br), 1H), 7.10 (d, *J* = 8.7 Hz, 2H), 6.84 (d, *J* = 8.7 Hz, 2H), 5.17-5.10 (m, 1H, OC*H*Me), 3.79 (s, 3H), 3.05 (s, 3H), 2.89 (dd, *J* = 14, 7.0 Hz, 1H), 2.80 (dd, *J* = 14, 6.1 Hz, 1H), 1.31 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 158.7, 155.4, 130.6, 128.7, 114.1, 76.0, 55.4, 41.4, 36.3, 19.6; IR (neat) 3221, 3040, 3023, 2982, 2959, 2939, 2919, 2838, 1767, 1612, 1587, 1512, 1463, 1415, 1363, 1323, 1304, 1245, 1215, 1178, 1122, 1099, 1080, 1028, 969, 911, 854, 841, 828, 803, 785, 753, 734, 713 cm^{-1}; HMRS (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_{12}H_{17}NNaO_6S$ 326.0669; found 326.0681.



S35

(±)-1-(4-Bromophenyl)propan-2-yl *N*-methylsulfonyloxycarbamate (S35). The title compound was prepared according to general procedure C starting from 1-(4-bromophenyl)propan-2-ol[12] (3.40 g, 15.8 mmol). *N*-Mesyloxycarbamate **S35** was obtained as a white solid (1.43 g, 4.06 mmol, 26% yield over 2 steps) after flash chromatography on silica gel eluting with 25% EtOAc/hexanes. R$_f$ 0.35 (30% EtOAc/hexanes); mp 65-66 °C; ^{1}H NMR (500 MHz, CDCl$_3$) δ 8.05 (s (br), 1H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.07 (d, *J* = 8.5 Hz, 2H), 5.18-5.20 (m, 1H), 3.05 (s, 3H), 2.90 (dd, *J* = 14, 7.2 Hz, 1H), 2.82 (dd, *J* = 14, 5.9 Hz, 1H), 1.32 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 155.3, 135.7, 131.8, 131.3, 121.0, 75.3, 41.7, 36.3, 19.7; IR (neat) 3272, 3047, 3022, 3000, 2967, 2940, 1744, 1590, 1486, 1458, 1415, 1372, 1355, 1245, 1218, 1172, 1141, 1118, 1071, 1048, 973, 943, 916, 858, 838, 807, 767, 713, 705 cm^{-1}; HMRS (ESI-TOF) m/z: [M+NH$_4$]$^+$ calcd for $C_{11}H_{18}BrN_2O_5S$ 396.0114; found 369.0117.



S36

(±)-1-(4-(Trifluoromethyl)phenyl)propan-2-yl *N*-methylsulfonyloxycarbamate (S36). The title compound was prepared according to general procedure C starting from 1-(4-(trifluoromethyl)phenyl)propan-2-ol[10] (2.20 g, 10.8 mmol). *N*-Mesyloxycarbamate **S36** was obtained as a white solid (1.45 g, 4.25 mmol, 41% yield over 2 steps) after flash chromatography on silica gel eluting with 30% EtOAc/hexanes. R$_f$ 0.32 (30% EtOAc/hexanes); mp 62-63 °C; ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.16 (s (br), 1H), 7.57 (d, *J* = 8.0

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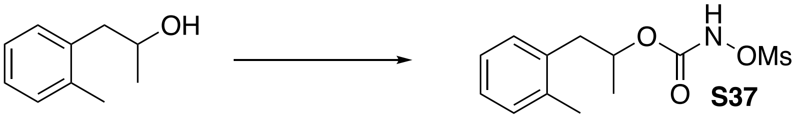
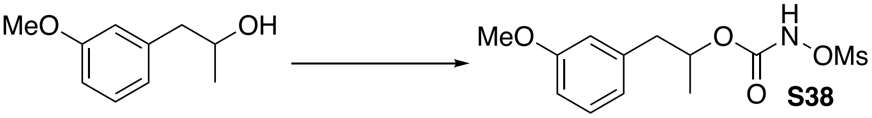
[12] A. Kaithal, B. Chatterjee and C. Gunanathan, *Org. Lett.*, 2015, **17**, 4790.

Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 5.25-5.15 (m, 1H), 3.03 (s, 3H), 3.01 (dd, *J* = 14, 7.3 Hz, 1H), 2.93 (dd, *J* = 14, 5.8 Hz, 1H), 1.34 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 155.2, 140.7, 129.8, 129.2 (d, *J* = 33 Hz), 125.5 (q, *J* = 3.6 Hz), 124.1 (q, *J* = 272 Hz), 75.0, 41.9, 36.1, 19.6; ^{19}F NMR (282 MHz, CDCl$_3$) δ (ppm) -63.9; IR (neat) 3421, 3321, 3271, 3205, 3046, 3021, 2998, 2978, 2937, 1745, 1680, 1613, 1587, 1460, 1415, 1375, 1357, 1321, 1247, 1219, 1168, 1114, 1065, 1016, 973, 916, 863, 816, 787, 767, 733, 707 cm^{-1}; HMRS (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_{12}H_{14}F_3NNaO_5S$ 364.0437; found 364.0436.



(±)-1-*o*-Tolylpropan-2-yl *N*-methylsulfonyloxycarbamate (*S*37). The title compound was prepared according to general procedure C starting from 1-(*o*-tolyl)propan-2-ol[10] (2.00 g, 13.3 mmol). *N*-Mesyloxycarbamate **S37** was obtained as a sticky oil (1.85 g, 6.44 mmol, 50% yield over 2 steps) after flash chromatography on silica gel eluting with 20% EtOAc/hexanes. R$_f$ 0.37 (30% EtOAc/hexanes); ^{1}H NMR (500 MHz, CDCl$_3$) δ 8.02 (s (br), 1H), 7.17-7.10 (m, 4H), 5.24-5.17 (m, 1H), 3.03 (s, 3H), 3.01 (dd, *J* = 14, 7.6 Hz, 1H), 2.84 (dd, *J* = 14, 6.3 Hz, 1H), 2.35 (s, 3H), 1.35 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 155.4, 136.8, 135.1, 130.6, 130.4, 127.2, 126.1, 75.1, 39.7, 36.3, 20.0, 19.7; IR (neat) 3284, 3020, 2983, 2938, 2874, 1738, 1459, 1414, 1369, 1325, 1246, 1180, 1134, 1091, 1076, 1051, 1029, 968, 799, 767, 744, 718 cm^{-1}; HMRS (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_{12}H_{17}NNaO_5S$ 310.0720; found 310.0719.



(±)-1-(3-methoxyphenyl)propan-2-yl *N*-methylsulfonyloxycarbamate (S38). The title compound was prepared according to general procedure C starting from 1-(3-methoxyphenyl)propan-2-ol[13] (1.55 g, 9.33 mmol) without DBU. *N*-Mesyloxycarbamate **S38** was obtained as pale yellow oil (1.65 g, 5,43 mmol, 53% over 2 steps) after flash chromatogramphy on silica gel eluting with 30% EtOAc/hexanes. R$_f$ 0.26 (30% EtOAc/hexanes); ^{1}H NMR (500 MHz, CDCl$_3$) δ 7.98 (s (br), 1H), 7.23-7.20 (m, 1H), 6.78 (dd, *J* = 7.9, 2.1 Hz, 2H), 6.75-6.71 (m, 1H), 5.22-5.16 (m, 1H), 3.80 (s, 3H), 3.05 (s, 3H), 2.93 (dd, *J* = 14, 7.2 Hz, 1H), 2.83 (dd, *J* = 14, 6.0 Hz, 1H), 1.33 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 159.8, 155.4, 138.3, 129.7, 121.9, 115.3, 112.2, 75.7, 55.3, 42.3, 36.0, 19.8; IR (neat) 3274, 3020, 2981, 2939, 2839, 1734, 1600, 1585, 1490, 1454, 1413, 1369, 1318, 1295, 1258, 1218, 1182, 1155, 1115, 1041, 967, 911, 878, 861, 805, 772, 742 cm^{-1}; (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_{12}H_{17}NNaO_6S$ 326.0669; found 326.0685.

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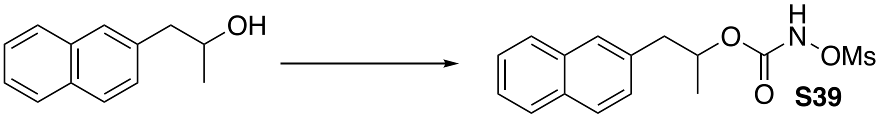
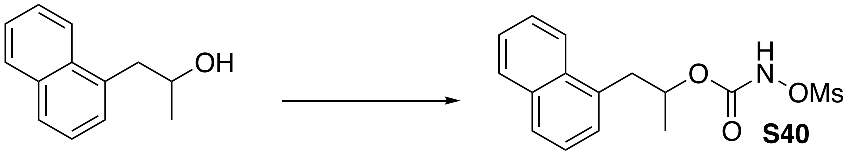
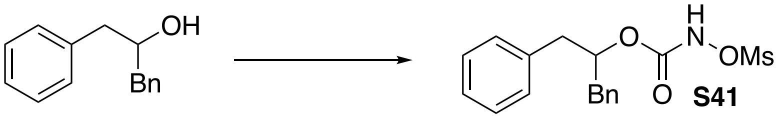
[13] X.-Y. Lu, C.-T. Yang, J.-H. Liu, Z.-Q. Zhang, X. Lu, X. Lou, B. Xiao and Y. Fu, *Chem. Commun.*, 2015, **51**, 2388.


S39

(±)-1-(Naphthalen-2-yl)propan-2-yl *N*-methylsulfonyloxycarbamate (S39). The title compound was prepared according to general procedure C starting from 1-(naphthalen-2-yl)propan-2-ol (1.15 g, 6.17 mmol). *N*-Mesyloxycarbamate **S39** was obtained as a white solid (1.02 g, 51% yield over 2 steps) after flash chromatography on silica gel eluting with 30% EtOAc/hexanes. R$_f$ 0.29 (30% EtOAc/hexanes); mp 78-80 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (s (br), 1H), 7.82-7.78 (m, 3H), 7.65 (s, 1H), 7.51-7.43 (m, 2H), 7.34 (dd, *J* = 8.4, 1.7 Hz, 1H), 5.34-5.26 (m, 1H), 3.12 (dd, *J* = 14, 7.3 Hz, 1H), 3.03 (dd, *J* = 14, 6.0 Hz, 1H), 2.86 (s, 3H), 1.37 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.3, 134.2, 133.5, 132.5, 128.3, 128.2, 127.74, 127.69, 127.67, 126.4, 125.9, 75.6, 42.5, 36.0, 19.8; IR (neat) 3249, 3044, 3016, 2993, 2935, 1724, 1630, 1597, 1507, 1484, 1459, 1410, 1371, 1328, 1272, 1184, 1153, 1140, 1101, 1046, 1015, 977, 920, 902, 862, 814, 799, 751 cm^{-1}; HMRS (ESI-TOF) m/z: $[M+NH_4]^+$ calcd for $C_{15}H_{21}N_2O_5S$ 341.1166; found 341.1170.


S40

(±)-1-(Naphthalen-1-yl)propan-2-yl *N*-methylsulfonyloxycarbamate (S40). The title compound was prepared according to general procedure C starting from 1-(naphthalen-1-yl)propan-2-ol[14] (0.89 g, 4.76 mmol). *N*-Mesyloxycarbamate **S40** was obtained as a white solid (1.20 g, 78% yield over 2 steps) after flash chromatography on silica gel eluting with 30% EtOAc/hexanes. R$_f$ 0.31 (30% EtOAc/hexanes); mp 78-80 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.5 Hz, 1H), 7.93 (s (br), 1H), 7.86 (d, *J* = 7.9 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.58-7.55 (m, 1H), 7.52-7.49 (m, 1H), 7.43-7.40 (m, 1H), 7.34 (d, *J* = 6.9 Hz, 1H), 5.39-5.33 (m, 1H), 3.55 (dd, *J* = 14, 6.8 Hz, 1H), 3.21 (dd, *J* = 14, 6.9 Hz, 1H), 3.00 (s, 3H), 1.36 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.4, 134.0, 132.9, 132.2, 129.0, 128.03, 127.97, 126.5, 126.0, 125.5, 123.8, 75.5, 39.5, 36.3, 20.0; IR (neat) 3238, 3049, 3020, 2994, 2985, 2956, 2938, 1724, 1595, 1486, 1462, 1447, 1409, 1373, 1327, 1299, 1262, 1188, 1139, 1101, 1044, 1015, 976, 908, 872, 848, 797, 780, 753 cm^{-1}; HMRS (ESI-TOF) m/z: $[M+Na]^+$calcd for $C_{15}H_{17}NNaO_5S$ 346.0720; found 346.0729.


S41

(±)-1,3-Diphenylpropan-2-yl *N*-mesyloxycarbamate (S41). The title compound was prepared according to general procedure C starting from 1,3-diphenylpropan-2-yl (2.97 g, 14.0 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (3.19 g, 11.7 mmol, 84% yield). The mesylation of the *N*-hydroxycarbamate (1.60 g, 5.89 mmol) afforded **S41** (1.34 g, 3.84 mmol, 65% yield) as a viscous oil after flash chromatography on silica gel eluting with 20% AcOEt/hexanes. R$_f$ 0.78 (40% EtOAc/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$)

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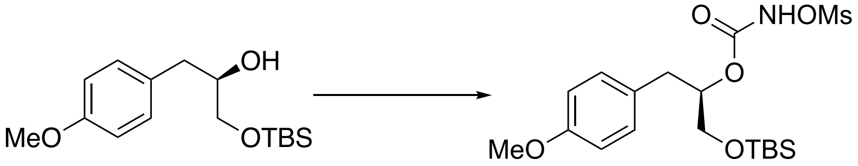
[14] H. Inui and S. Murata, *J. Am. Chem. Soc.*, 2005, **127**, 2628.

δ 7.89 (s (br), 1H), 7.32-7.29 (m, 4H), 7.25-7.22 (m, 2H), 7.21-7.19 (m, 4H), 5.41-5.36 (m, 1H), 2.99-2.91 (m, 4H), 2.82 (s, 3H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 155.0, 136.4, 129.4, 128.6, 126.9, 79.0, 40.2, 35.9; IR (neat) 3284, 1743, 1373, 1181, 700, 506 cm^{-1}; HRMS (ESI-TOF) m/z: [M+Na]$^+$ calcd for $C_{17}H_{19}NNaO_5S$ 372.0876; found 372.0867.



(*R*)-52

(*R*)-1-((*tert*-Butyldimethylsilyl)oxy)-3-(4-methoxyphenyl)propan-2-yl *N*-mesyloxy-carbamate (52). The title compound was prepared according to general procedure B starting from (*R*)-1-((*tert*-butyldimethylsilyl)oxy)-3-(4-methoxyphenyl)propan-2-ol[15] (2.64 g, 8.91 mmol). The crude *N*-hydroxycarbamate was isolated as a white solid (1.67 g, 4.70 mmol, 53% yield). The mesylation of the *N*-hydroxycarbamate (990 mg, 2.78 mmol) afforded **52** (772 mg, 1.78 mmol, 64% yield) as a viscous oil after flash chromatography on silica gel eluting with 20% AcOEt/Hexanes. R$_f$ 0.39 (20% AcOEt/hexanes); $[\alpha]^{25}_{D}$ -22.7 (c 1.00, MeOH); ^{1}H NMR (500 MHz, CDCl$_3$) δ 8.19 (s (br), 1H), 7.14-7.11 (m, 2H), 6.85-6.82 (m, 2H), 5.09-5.05 (m, 1H), 3.78 (s, 3H), 3.71 (dd, *J* = 11 Hz, 4.0 Hz, 1H), 3.65 (dd, *J* = 11.2, 5.4 Hz, 1H), 3.04 (s, 3H), 2.94 (dd, *J* = 14 Hz, 6.2 Hz, 1H), 2.85 (dd, *J* = 14 Hz, 7.4 Hz, 1H), 0.90 (s, 9H), 0.05 (s, 6H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 158.6, 155.9, 130.4, 127.9, 114.1, 79.3, 63.1, 55.2, 36.1, 35.7, 25.6, 17.9, -3.63; IR (neat) 3280, 2950, 2930, 2856, 1739, 1612, 1411, 1512, 1245, 1177, 1030, 969, 860, 807, 505 cm^1; HRMS (ESI-TOF) m/z: [M+H]$^+$ calcd for $C_{18}H_{32}NO_7SSi$ 434.1663; found 434.1675.

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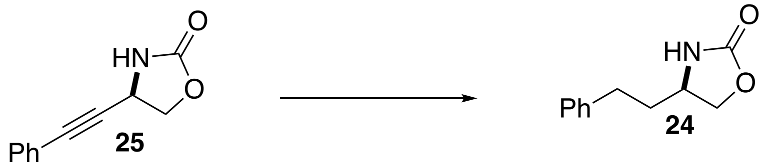
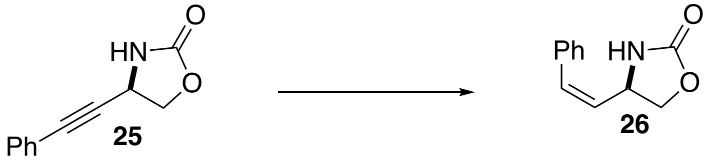
[15] S. V. Narina, T. S. Kumar, S. George and A. Sudalai, *Tetrahedron Lett.*, 2007, **48**, 65.

Hydrogenation of Oxazolidinone 25



4-Phenethyloxazolidin-2-one (24).[16] In a 25 mL round-bottom flask, equipped with a magnetic stirbar, Pd/C 10% catalyst (5.0 mg, 10% wt.) was suspended in MeOH (2.5 mL, 0.1 M). Oxazolidinone **25** (46.8 mg, 0.25 mmol, 1.00 equiv) was added. Hydrogen was bubbled into the suspension twice using hydrogen balloons (connected with needles). A hydrogen balloon was connected to the reaction flask and the suspension was stirred 12 h at rt. The reaction was monitored by TLC (40% EtOAc/Hexanes). The reaction mixture was filtered through celite and the cake was thoroughly washed with MeOH. The solvent was removed under reduced pressure and the residue was chromatographed on silica gel (solid sample) eluting with 40% EtOAc/Hexanes to afford the title compound as white crystals (46 mg, 0.24 mmol, 96% yield).



(*Z*)-4-Styryloxazolidin-2-one (26). In a 25 mL round-bottom flask, equipped with a magnetic stirbar, Lindlar's catalyst (18.8 mg, 40% wt.) was suspended in EtOAc (2.5 mL, 0.1 M). Oxazolidinone **25** (46.8 mg, 0.25 mmol, 1.00 equiv) was added followed by quinoline (distilled under argon over Zn powder) (0.590 mL, 5.00 mmol, 20.0 equiv). Hydrogen was bubbled into the suspension twice using hydrogen balloons (connected with needles). A hydrogen balloon was connected to the reaction flask and the suspension was stirred at rt for 1 hour. The reaction was monitored by TLC (40% EtOAc/Hexanes). The reaction mixture was filtered through celite and the cake was thoroughly washed with EtOAc. The organic layer (25 mL) was washed with a 1,2 N HCl aqueous solution (15 mL). The organic layer was washed with water (15 mL) and brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was chromatographed on silica gel (solid sample) eluting with 40% EtOAc/Hexanes 4 : 6 to afford the title compound as white crystals (46 mg, 0.24 mmol, 96% yield). R_f 0.26 (40% EtOAc/Hexanes); mp 120.5-122.0 °C (lit. 90-91 °C);[17] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39-7.27 (m, 3H), 7.12 (d, *J* = 7.5 Hz, 2H), 6.71 (d, *J* = 11.5 Hz, 1H), 6.45 (br (s), 1H), 5.68 (dd, *J* = 11.5, 9.0 Hz, 1H), 4.81 (q, *J* = 8.5 Hz, 1H), 4.55 (t, *J* = 8.5 Hz, 1H), 4.12 (dd, *J* = 8.5 Hz, 7.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.9, 135.3, 134.0, 129.3, 128.5, 128.3, 127.8, 70.3, 50.2.

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[17] M. P. Sibi, D. Rutherford, P. A. Renhowe and B. Li, *J. Am. Chem. Soc.*, 1999, **121**, 7509.

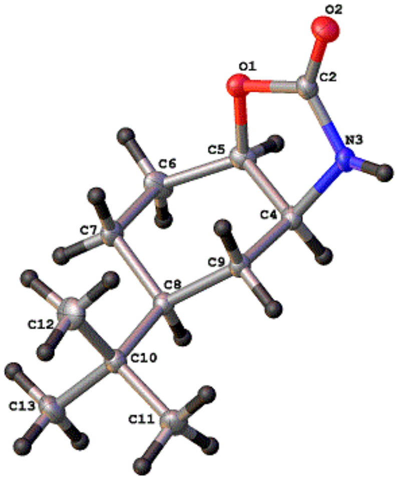

Table S4. Crystal data and structure refinement for Oxazolidinone *cis*-34.

Identification code	Oxazolidinone cis-34
Empirical formula	$C_{11}H_{19}NO_2$
Formula weight	197.27
Temperature/K	150
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.0400(4)
b/Å	6.0462(2)
c/Å	12.0358(3)
α/°	90
β/°	93.0384(11)
γ/°	90
Volume/Å^3	1092.93(5)
Z	4
ρ_{calc}g/cm^3	1.199
μ/mm^{-1}	0.419
F(000)	432.0
Crystal size/mm^3	0.3 × 0.06 × 0.04
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	5.12 to 121.202
Index ranges	$-19 \le h \le 19$, $-7 \le k \le 7$, $-15 \le l \le 15$
Reflections collected	18135
Independent reflections	2496 [R_{int} = 0.0348, R_{sigma} = 0.0192]
Data/restraints/parameters	2496/0/135
Goodness-of-fit on F^2	1.099
Final R indexes [I>=2σ (I)]	R_1 = 0.0481, wR_2 = 0.1186
Final R indexes [all data]	R_1 = 0.0516, wR_2 = 0.1223
Largest diff. peak/hole / e Å^{-3}	0.34/-0.40

Table S5. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for *cis*-34. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	6230.0(5)	717.3(13)	5353.9(6)	19.0(2)
O2	5473.4(6)	-535.2(14)	6791.0(7)	23.7(2)
C2	5702.9(7)	1022.3(19)	6230.0(8)	16.9(3)
N3	5511.3(6)	3182.4(16)	6330.9(8)	17.2(2)
C4	6102.7(7)	4504.2(18)	5667.6(8)	15.4(2)
C5	6248.4(7)	2823.4(18)	4752.4(8)	17.7(3)
C6	7099.8(8)	3079(2)	4146.2(9)	22.0(3)
C7	7909.5(7)	3755.4(19)	4889.5(9)	18.6(3)
C8	7713.5(6)	5778.0(17)	5604.8(8)	14.5(2)
C9	6955.3(6)	5139.8(18)	6345.7(8)	14.9(2)
C10	8550.6(7)	6709.8(18)	6264.4(9)	17.9(3)
C11	8277.1(8)	8528(2)	7067(1)	24.0(3)
C12	9055.1(8)	4912(2)	6940.9(10)	27.1(3)
C13	9180.1(8)	7739(2)	5442.0(11)	27.4(3)

Table S6. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for *cis*-34. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	22.8(4)	17.2(4)	17.5(4)	-1.9(3)	7.6(3)	-1.6(3)
O2	25.9(4)	21.1(5)	24.9(4)	3.7(3)	8.8(3)	-3.3(3)
C2	14.5(5)	20.2(6)	16.0(5)	-0.9(4)	2.6(4)	-2.3(4)
N3	14.9(4)	18.7(5)	18.5(5)	-1.2(3)	6.2(3)	-0.6(3)
C4	13.8(5)	16.9(5)	15.8(5)	1.7(4)	1.8(4)	0.7(4)
C5	20.8(5)	19.7(6)	12.5(5)	0.6(4)	0.5(4)	-3.3(4)
C6	27.6(6)	27.3(6)	11.8(5)	-3.7(4)	6.2(4)	-6.6(5)
C7	19.4(5)	20.8(6)	16.3(5)	-2.2(4)	6.9(4)	-0.5(4)
C8	14.8(5)	15.5(5)	13.1(5)	1.3(4)	2.2(4)	0.7(4)
C9	15.4(5)	17.1(5)	12.3(4)	-1.9(4)	2.2(3)	0.0(4)
C10	15.1(5)	18.2(5)	20.4(5)	-0.5(4)	1.8(4)	-0.9(4)
C11	23.1(6)	23.0(6)	26.0(6)	-7.4(5)	2.0(4)	-4.8(4)
C12	19.5(5)	30.9(7)	30.1(6)	2.4(5)	-6.2(4)	3.5(5)
C13	21.5(6)	28.0(7)	33.6(6)	-1.7(5)	8.8(5)	-6.9(5)

Table S7. Bond Lengths *cis*-34.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C2	1.3649(12)	C6	C7	1.5282(15)
O1	C5	1.4657(13)	C7	C8	1.5332(14)
O2	C2	1.2192(13)	C8	C9	1.5336(13)

C2	N3	1.3444(15)	C8	C10	1.5579(14)
N3	C4	1.4638(13)	C10	C11	1.5340(15)
C4	C5	1.5230(14)	C10	C12	1.5342(16)
C4	C9	1.5320(14)	C10	C13	1.5371(15)
C5	C6	1.5149(15)			

Table S8. Bond Angles for *cis*-34.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	O1	C5	106.93(8)	C6	C7	C8	111.80(9)
O2	C2	O1	121.10(10)	C7	C8	C9	107.27(8)
O2	C2	N3	129.20(10)	C7	C8	C10	113.60(8)
N3	C2	O1	109.70(9)	C9	C8	C10	113.61(8)
C2	N3	C4	109.99(8)	C4	C9	C8	112.37(8)
N3	C4	C5	98.34(8)	C11	C10	C8	110.09(9)
N3	C4	C9	111.23(8)	C11	C10	C12	108.37(9)
C5	C4	C9	113.84(8)	C11	C10	C13	108.07(9)
O1	C5	C4	102.43(8)	C12	C10	C8	112.20(9)
O1	C5	C6	111.41(9)	C12	C10	C13	108.93(10)
C6	C5	C4	115.98(9)	C13	C10	C8	109.09(9)
C5	C6	C7	114.40(8)				

Table S9. Hydrogen Bonds for *cis*-34.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N3	H3	O2[1]	0.859(16)	2.022(17)	2.8738(12)	171.3(15)

[1] 1-X,1/2+Y,3/2-Z

Table S10. Torsion Angles for *cis*-34.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C2	N3	C4	-14.27(12)	C5	C6	C7	C8	-50.73(13)
O1	C5	C6	C7	-78.31(12)	C6	C7	C8	C9	60.89(11)
O2	C2	N3	C4	165.71(11)	C6	C7	C8	C10	-172.70(9)
C2	O1	C5	C4	28.21(10)	C7	C8	C9	C4	-60.73(11)
C2	O1	C5	C6	152.84(9)	C7	C8	C10	C11	-172.76(9)
C2	N3	C4	C5	30.29(11)	C7	C8	C10	C12	-51.98(12)
C2	N3	C4	C9	-89.39(10)	C7	C8	C10	C13	68.82(11)
N3	C4	C5	O1	-33.80(9)	C9	C4	C5	O1	83.90(10)
N3	C4	C5	C6	-155.35(9)	C9	C4	C5	C6	-37.65(13)
N3	C4	C9	C8	159.75(9)	C9	C8	C10	C11	-49.77(12)
C4	C5	C6	C7	38.33(14)	C9	C8	C10	C12	71.01(12)
C5	O1	C2	O2	170.30(10)	C9	C8	C10	C13	-168.19(9)
C5	O1	C2	N3	-9.71(11)	C10	C8	C9	C4	172.87(9)
C5	C4	C9	C8	49.77(12)					

Table S11. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for *cis*-34.

Atom	*x*	*y*	*z*	U(eq)
H3	5263(11)	3660(30)	6910(13)	28(4)
H4	5790	5848	5360	19
H5	5730	2878	4197	21
H6A	7003	4203	3555	26
H6B	7232	1658	3781	26
H7A	8412	4098	4419	22
H7B	8090	2503	5381	22
H8	7484	6971	5091	17
H9A	7148	3878	6824	18
H9B	6827	6401	6837	18
H11A	7860	9545	6676	36
H11B	8807	9346	7341	36
H11C	7989	7856	7696	36
H12A	8648	4182	7434	41
H12B	9547	5588	7387	41
H12C	9292	3819	6433	41
H13A	9371	6599	4928	41
H13B	9702	8357	5854	41
H13C	8868	8918	5021	41

Experimental

Single crystals of $C_{11}H_{19}NO_2$ **(*cis*-34)** were obtained from a $CDCl_3$ solution. A suitable crystal was selected and mounted on a Bruker Venture Metaljet diffractometer. The crystal was kept at 150 K during data collection. Using Olex2[18], the structure was solved with the ShelXT[19] structure solution program using Direct Methods and refined with the XL[20]refinement package using Least Squares minimization.

Crystal structure determination of oxazolidinone *cis*-34

Crystal Data for $C_{11}H_{19}NO_2$ (M =197.27 g/mol): monoclinic, space group P2$_1$/c (no. 14), a = 15.0400(4) Å, b = 6.0462(2) Å, c = 12.0358(3) Å, β = 93.0384(11)°, V = 1092.93(5) Å^3, Z = 4, T = 150 K, μ(GaKα) = 0.419 mm^{-1}, $Dcalc$ = 1.199 g/cm^3, 18135 reflections measured (5.12° ≤ 2Θ ≤ 121.202°), 2496 unique (R_{int} = 0.0348, R_{sigma} = 0.0192) which were used in all calculations. The final R_1 was 0.0481 (I > 2σ(I)) and wR_2 was 0.1223 (all data).

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[18] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339.

[19] G. M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3.

[20] G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112.

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:
1. Fixed Uiso

At 1.2 times of:

All C(H) groups, All C(H,H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Ternary CH refined with riding coordinates:

C4(H4), C5(H5), C8(H8)

2.b Secondary CH2 refined with riding coordinates:

C6(H6A,H6B), C7(H7A,H7B), C9(H9A,H9B)

2.c Idealised Me refined as rotating group:

C11(H11A,H11B,H11C), C12(H12A,H12B,H12C), C13(H13A,H13B,H13C)

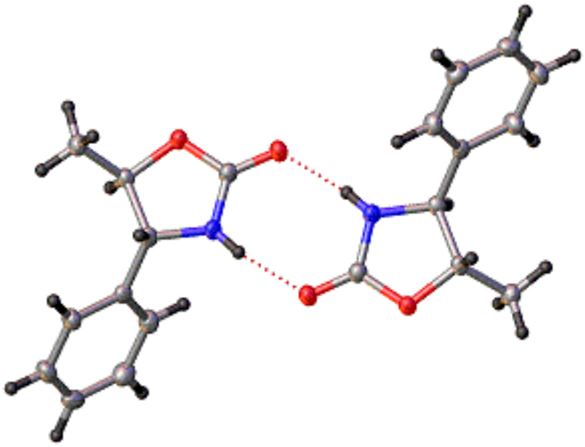

Table S12. Crystal data and structure refinement for *trans*-40.

Identification code	*trans*-**40**
Empirical formula	$C_{10}H_{11}NO_2$
Formula weight	177.20
Temperature/K	100
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	14.32966(13)
b/Å	8.77119(8)
c/Å	14.61018(13)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1836.33(3)
Z	8
ρ_{calc}g/cm^3	1.282
μ/mm^{-1}	0.735
F(000)	752.0
Crystal size/mm^3	0.2 × 0.18 × 0.16
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	11.83 to 143.922
Index ranges	$-17 \le h \le 17$, $-10 \le k \le 10$, $-18 \le l \le 17$
Reflections collected	23996
Independent reflections	3449 [R_{int} = 0.0221, R_{sigma} = 0.0140]
Data/restraints/parameters	3449/1/245
Goodness-of-fit on F^2	1.061
Final R indexes [I>=2σ (I)]	R_1 = 0.0279, wR_2 = 0.0738
Final R indexes [all data]	R_1 = 0.0281, wR_2 = 0.0742
Largest diff. peak/hole / e Å^{-3}	0.23/-0.22
Flack parameter	0.00(4)

Table S13. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for *trans*-40. U$_{eq}$ is defined as 1/3 of of the trace of the orthogonalised U$_{IJ}$ tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	2989.9(8)	7256.3(14)	3349.8(9)	24.5(3)
O2	4180.0(8)	6017.3(15)	4014.7(9)	26.5(3)
N3	2647.3(10)	5461.6(17)	4356.0(11)	23.5(3)
C2	3337.7(12)	6207.6(19)	3930.3(12)	21.6(3)
C4	1741.2(11)	6158.1(19)	4193.3(12)	20.2(3)
C5	1971.2(11)	7162.5(19)	3349.8(12)	20.1(3)
C6	1578.3(12)	8758.1(19)	3395.9(14)	25.3(4)
C7	966.1(11)	5021(2)	4023.5(11)	19.9(3)
C8	1138.5(12)	3599(2)	3638.7(13)	26.1(4)
C9	410.7(13)	2580(2)	3486.7(14)	30.7(4)
C10	-497.4(13)	2977(2)	3713.3(14)	29.6(4)
C11	-676.6(12)	4399(2)	4078.9(14)	30.4(4)
C12	51.0(12)	5418(2)	4240.2(14)	25.5(4)
O21	4452.1(8)	2622.9(14)	6587.2(8)	22.7(3)
O22	3256.5(8)	3801.0(14)	5900.2(9)	26.9(3)
N23	4781.5(10)	4541.3(16)	5658.3(11)	22.7(3)
C22	4096.4(12)	3682.7(18)	6021.4(12)	21.2(3)
C24	5698.3(11)	3895.7(18)	5844.2(12)	19.3(3)
C25	5461.3(10)	2839.3(18)	6659.7(12)	19.0(3)
C26	5928.6(12)	1301.0(19)	6637.2(14)	24.2(4)
C27	6443.1(11)	5073.0(19)	6063.3(11)	19.6(3)
C28	6225.9(12)	6477(2)	6445.1(13)	25.2(4)
C29	6928.4(13)	7525(2)	6639.0(14)	29.2(4)
C30	7851.3(13)	7168(2)	6462.8(13)	28.5(4)
C31	8075.4(12)	5759(2)	6103.2(16)	31.8(4)
C32	7373.5(12)	4717(2)	5897.0(13)	26.4(4)

Table S14. Anisotropic Displacement Parameters (Å^2×10^3) for *trans*-40. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	17.5(6)	29.8(6)	26.1(6)	9.9(5)	1.5(5)	2.7(5)
O2	17.3(5)	33.4(6)	28.9(7)	9.4(5)	-0.1(5)	1.8(5)
N3	18.0(7)	30.7(8)	21.7(7)	10.4(6)	-3.3(6)	0.2(5)
C2	21.2(8)	24.4(8)	19.1(8)	3.4(6)	-1.2(6)	0.9(6)
C4	18.1(7)	25.8(8)	16.7(8)	1.9(6)	-0.5(6)	1.4(6)
C5	16.4(7)	25.0(7)	19.0(8)	1.5(7)	0.1(6)	1.0(6)
C6	23.5(8)	24.4(8)	28.1(9)	1.4(7)	-1.0(7)	2.4(6)

C7	19.5(8)	24.8(8)	15.4(8)	4.3(6)	-0.8(6)	-0.2(6)
C8	23.6(8)	30.6(9)	24.0(9)	-0.9(7)	-0.7(7)	3.2(7)
C9	35.7(9)	25.6(9)	30.8(11)	-0.9(8)	-7.4(8)	0.2(7)
C10	29.1(9)	32.3(10)	27.3(9)	7.8(8)	-6.3(7)	-9.7(7)
C11	18.5(8)	38.9(10)	33.6(10)	5.4(8)	0.9(7)	-1.5(7)
C12	19.6(8)	28.5(9)	28.5(10)	1.5(7)	1.0(7)	1.6(6)
O21	17.1(6)	27.2(6)	23.8(6)	7.7(5)	-0.2(5)	0.0(4)
O22	17.5(6)	33.2(6)	30.1(7)	9.9(5)	-1.5(5)	-0.2(5)
N23	18.3(7)	27.8(7)	22.0(8)	8.9(6)	-2.6(6)	-0.7(5)
C22	20.9(8)	23.5(7)	19.3(8)	2.3(6)	-0.2(6)	1.4(6)
C24	17.8(7)	23.1(7)	16.9(8)	0.5(6)	0.3(6)	1.2(6)
C25	15.5(7)	24.1(8)	17.4(8)	-0.3(7)	-0.6(6)	0.3(5)
C26	24.1(8)	23.6(8)	24.8(9)	0.0(7)	-0.6(7)	3.3(6)
C27	18.9(7)	23.9(8)	16.1(8)	4.7(6)	-0.6(6)	0.8(6)
C28	22.4(8)	26.5(8)	26.8(9)	-1.6(7)	-0.3(7)	4.2(6)
C29	34.8(9)	22.0(8)	30.8(10)	-1.6(7)	-4.0(8)	2.3(7)
C30	28.9(9)	29.2(9)	27.3(10)	4.4(7)	-4.9(8)	-8.1(7)
C31	19.2(8)	37.3(10)	39.0(11)	-0.3(8)	0.9(8)	-1.6(7)
C32	21.5(8)	25.5(8)	32.1(10)	-2.2(7)	2.8(7)	1.4(6)

Table S15. Bond Lengths for *trans*-40.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C2	1.347(2)	O21	C22	1.344(2)
O1	C5	1.4621(18)	O21	C25	1.4625(17)
O2	C2	1.225(2)	O22	C22	1.221(2)
N3	C2	1.339(2)	N23	C22	1.346(2)
N3	C4	1.454(2)	N23	C24	1.456(2)
C4	C5	1.550(2)	C24	C25	1.547(2)
C4	C7	1.513(2)	C24	C27	1.519(2)
C5	C6	1.510(2)	C25	C26	1.507(2)
C7	C8	1.390(3)	C27	C28	1.387(2)
C7	C12	1.393(2)	C27	C32	1.391(2)
C8	C9	1.391(3)	C28	C29	1.393(3)
C9	C10	1.387(3)	C29	C30	1.383(3)
C10	C11	1.381(3)	C30	C31	1.381(3)
C11	C12	1.393(2)	C31	C32	1.392(3)

Table S16. Bond Angles for *trans*-40.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	O1	C5	109.33(12)	C22	O21	C25	109.25(12)
C2	N3	C4	112.23(14)	C22	N23	C24	111.52(13)
O2	C2	O1	121.41(15)	O21	C22	N23	110.65(14)

O2	C2	N3	127.93(16)	O22	C22	O21	121.44(15)
N3	C2	O1	110.66(14)	O22	C22	N23	127.89(16)
N3	C4	C5	100.30(12)	N23	C24	C25	100.29(12)
N3	C4	C7	113.91(14)	N23	C24	C27	114.13(13)
C7	C4	C5	113.59(14)	C27	C24	C25	113.52(14)
O1	C5	C4	104.14(12)	O21	C25	C24	103.83(12)
O1	C5	C6	108.67(13)	O21	C25	C26	108.77(13)
C6	C5	C4	114.33(15)	C26	C25	C24	114.97(14)
C8	C7	C4	121.81(15)	C28	C27	C24	122.04(15)
C8	C7	C12	118.90(16)	C28	C27	C32	118.99(16)
C12	C7	C4	119.28(15)	C32	C27	C24	118.95(15)
C7	C8	C9	120.51(16)	C27	C28	C29	120.38(16)
C10	C9	C8	120.25(18)	C30	C29	C28	120.25(17)
C11	C10	C9	119.57(17)	C31	C30	C29	119.73(17)
C10	C11	C12	120.38(17)	C30	C31	C32	120.13(17)
C7	C12	C11	120.37(17)	C27	C32	C31	120.50(17)

Table S17. Hydrogen Bonds for *trans*-40.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N3	H3	O22	0.83(3)	2.00(3)	2.8238(19)	171(2)
N23	H23	O2	0.84(3)	2.02(3)	2.861(2)	172(2)

Table S18. Torsion Angles for *trans*-40.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N3	C4	C5	O1	-17.22(17)	N23	C24	C25	O21	19.98(15)
N3	C4	C5	C6	-135.66(14)	N23	C24	C25	C26	138.67(14)
N3	C4	C7	C8	-28.5(2)	N23	C24	C27	C28	27.0(2)
N3	C4	C7	C12	152.89(16)	N23	C24	C27	C32	-154.66(16)
C2	O1	C5	C4	13.19(18)	C22	O21	C25	C24	-15.52(16)
C2	O1	C5	C6	135.44(16)	C22	O21	C25	C26	-138.38(15)
C2	N3	C4	C5	16.89(18)	C22	N23	C24	C25	-19.25(18)
C2	N3	C4	C7	138.59(15)	C22	N23	C24	C27	-140.97(16)
C4	N3	C2	O1	-9.8(2)	C24	N23	C22	O21	10.8(2)
C4	N3	C2	O2	170.87(18)	C24	N23	C22	O22	-170.53(17)
C4	C7	C8	C9	-179.70(17)	C24	C27	C28	C29	179.80(17)
C4	C7	C12	C11	179.15(17)	C24	C27	C32	C31	-178.96(18)
C5	O1	C2	O2	176.46(15)	C25	O21	C22	O22	-174.94(16)
C5	O1	C2	N3	-2.9(2)	C25	O21	C22	N23	3.82(19)
C5	C4	C7	C8	85.57(19)	C25	C24	C27	C28	-87.14(19)
C5	C4	C7	C12	-93.09(18)	C25	C24	C27	C32	91.24(19)
C7	C4	C5	O1	-139.15(14)	C27	C24	C25	O21	142.13(13)

C7	C4	C5	C6	102.42(17)	C27	C24	C25	C26	-99.18(17)
C7	C8	C9	C10	0.4(3)	C27	C28	C29	C30	-0.8(3)
C8	C7	C12	C11	0.4(3)	C28	C27	C32	C31	-0.5(3)
C8	C9	C10	C11	0.9(3)	C28	C29	C30	C31	-0.8(3)
C9	C10	C11	C12	-1.5(3)	C29	C30	C31	C32	1.6(3)
C10	C11	C12	C7	0.8(3)	C30	C31	C32	C27	-1.0(3)
C12	C7	C8	C9	-1.0(3)	C32	C27	C28	C29	1.4(3)

Table S19. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for *trans*-40.

Atom	*x*	*y*	*z*	U(eq)
H3	2768(15)	4950(30)	4820(18)	30(6)
H4	1572	6825	4723	24
H5	1752	6647	2779	24
H6A	1787	9252	3962	38
H6B	895	8712	3388	38
H6C	1798	9347	2868	38
H8	1758	3321	3478	31
H9	536	1609	3227	37
H10	-993	2275	3618	36
H11	-1299	4684	4221	36
H12	-78	6389	4499	31
H23	4657(15)	5000(30)	5170(20)	34(6)
H24	5903	3266	5310	23
H25	5613	3367	7248	23
H26A	5731	703	7170	36
H26B	6607	1435	6652	36
H26C	5752	764	6075	36
H28	5594	6725	6575	30
H29	6773	8489	6893	35
H30	8329	7889	6589	34
H31	8710	5500	5996	38
H32	7531	3755	5641	32

Experimental

Single crystals of $C_{10}H_{11}NO_2$ (***trans*-40**) were obtained from a 20% $CHCl_3$/hexanes solution. A suitable crystal was selected and mounted on a Bruker Smart APEX diffractometer. The crystal was kept at 100 K during data collection. Using Olex2[18], the structure was solved with the ShelXT[19] structure solution program using Intrinsic Phasing and refined with the XL[20] refinement package using Least Squares minimization.

Crystal structure determination of *trans*-40

Crystal Data for $C_{10}H_{11}NO_2$ (M =177.20 g/mol): orthorhombic, space group Pna2_1 (no. 33), a = 14.32966(13) Å, b = 8.77119(8) Å, c = 14.61018(13) Å, V = 1836.33(3) Å^3, Z = 8, T = 100 K, μ(CuKα) = 0.735 mm^{-1}, $Dcalc$ = 1.282 g/cm^3, 23996 reflections measured (11.83° ≤ 2Θ ≤ 143.922°), 3449 unique (R_{int} = 0.0221, R_{sigma} = 0.0140) which were used in all calculations. The final R_1 was 0.0279 (I > 2σ(I)) and wR_2 was 0.0742 (all data).

Refinement model description

Number of restraints - 1, number of constraints - unknown.

Details:

1. Fixed Uiso

At 1.2 times of:

All C(H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Ternary CH refined with riding coordinates:

C4(H4), C5(H5), C24(H24), C25(H25)

2.b Aromatic/amide H refined with riding coordinates:

C8(H8), C9(H9), C10(H10), C11(H11), C12(H12), C28(H28), C29(H29), C30(H30),

C31(H31), C32(H32)

2.c Idealised Me refined as rotating group:

C6(H6A,H6B,H6C), C26(H26A,H26B,H26C)

Content: Cartesian coordinates, total energies (a.u), vibrational zero-point energies (a.u) and free energies (a.u, at 298.15 K, and 1 atm) for the stationary structures of rhodium nitrenes **A** and **B**, oxazolidinone **30, 33** and **35**.
The order of the stationary point is based on the number of imaginary frequency. All of the results shown here are from DFT calculations using PBEPBE functional, and the 6-31G(d) basis set was used for all the C, H, O and N atoms, the 1997 stuttgart relativistic small-core potential (Stuttgart RSC 1997 ECP) for Rh, augmented with 4f function (**ζ**f(Rh)=1.350). This basis set level is denoted as BS1 in this article.

- ***Cyclohexyloxynitrene species A-equatorial (A) (Figure 4)***

Rh	-0.560692	-0.266599	-0.449859
Rh	-2.542186	0.501996	0.713748
O	0.499600	0.012944	1.292413
O	-1.378014	0.744175	2.392030
O	-1.733141	-0.508466	-2.135687
O	-3.600663	0.223053	-1.016715
O	-0.271530	1.723015	-0.938706
O	-2.151937	2.416510	0.161651
O	-1.068670	-2.145999	0.190504
O	-2.940717	-1.410694	1.271432
C	-0.132775	0.451010	2.326444
C	-1.107748	2.619919	-0.554691
C	-2.984589	-0.223703	-2.050985
C	-2.124407	-2.327647	0.902820
N	0.973713	-0.805885	-1.445396
C	2.167570	-1.056265	-0.830840
O	2.430003	-2.234447	-0.531216
O	2.990083	0.005136	-0.689818
C	0.689286	0.608929	3.586115
H	0.879536	-0.386762	4.022730
H	1.665141	1.059608	3.346915
H	0.150548	1.224944	4.319810
C	-0.832442	4.031849	-1.014731
H	0.238170	4.264185	-0.905655
H	-1.084963	4.119205	-2.085566
H	-1.442352	4.744690	-0.441977
C	-2.408303	-3.748181	1.326141
H	-2.550579	-4.378502	0.432708
H	-1.542297	-4.151048	1.876268
H	-3.307372	-3.785537	1.956858
C	-3.809549	-0.470431	-3.294293
H	-3.224238	-0.227806	-4.193896
H	-4.074212	-1.541129	-3.343504
H	-4.736478	0.119977	-3.262351
C	4.334287	-0.283393	-0.182910
C	5.268264	-0.620762	-1.348792
C	4.790645	0.957748	0.583496
H	4.260571	-1.150715	0.497707
C	6.715359	-0.791499	-0.850747
H	5.217106	0.203497	-2.086103

H	4.911972	-1.537219	-1.850458
C	6.237643	0.784069	1.080319
H	4.726531	1.832158	-0.092513
H	4.099609	1.147248	1.424658
C	7.192608	0.450042	-0.078689
H	7.382813	-0.997631	-1.706650
H	6.772625	-1.678304	-0.188771
H	6.565328	1.700846	1.602902
H	6.272944	-0.033390	1.827806
H	7.240143	1.313995	-0.771002
H	8.217781	0.294104	0.3037647

- E(PBE-PBE) = -1612.23878562
- No imaginary frequency
- Zero-point correction = 0.380805
- Sum of electronic and thermal Enthalpies = -1611.824461
- Sum of electronic and thermal Free Energies = -1611.925670

TS-Cis Cyclohexyloxynitrene species A-equatorial (Figure 4)

Rh	-0.153534	-0.178382	-0.127665
Rh	-2.437578	0.541812	0.208532
O	-0.431564	-1.557672	1.366528
O	-2.604300	-0.883706	1.670166
O	0.017530	1.281713	-1.585237
O	-2.163540	1.932444	-1.274421
O	0.417597	1.193420	1.284312
O	-1.741392	1.878773	1.591323
O	-0.917531	-1.471749	-1.532768
O	-3.079268	-0.809116	-1.163851
C	-1.586895	-1.621324	1.930013
C	-0.486411	1.934861	1.831258
C	-1.017823	1.999208	-1.848512
C	-2.182189	-1.526094	-1.742075
N	1.677780	-0.743738	-0.502720
C	2.129634	-2.025630	-0.231523
O	1.524075	-3.038980	-0.561805
O	3.374216	-2.172746	0.389710
H	2.982731	0.007737	1.919064
C	-2.645119	-2.532282	-2.769976
H	-2.202154	-2.289304	-3.750108
H	-2.286938	-3.535993	-2.488892
H	-3.741502	-2.527827	-2.845288
C	-1.757467	-2.695043	2.980755
H	-2.631821	-2.479664	3.611314
H	-1.908478	-3.666437	2.478718
H	-0.847065	-2.776803	3.593983
C	-0.002768	2.970394	2.820431
H	0.432781	3.823502	2.271196
H	-0.841031	3.334627	3.431047
H	0.783900	2.547584	3.464528

C	-0.867848	3.003914	-2.970753
H	0.137571	3.451415	-2.952103
H	-0.985621	2.484316	-3.937716
H	-1.639422	3.783333	-2.893975
C	4.261418	-1.040204	0.445435
C	4.920022	-0.773304	-0.920694
C	3.551837	0.179028	0.994549
H	5.047286	-1.352496	1.167762
C	5.740361	0.527499	-0.901908
H	4.122089	-0.693233	-1.681987
H	5.543414	-1.642687	-1.190664
C	4.185243	1.530296	0.831358
H	2.453145	0.017826	-0.005880
C	4.853232	1.729296	-0.541156
H	6.214087	0.681959	-1.887530
H	6.566876	0.441746	-0.167465
H	3.445623	2.321977	1.048644
H	4.962756	1.625029	1.627062
H	5.441851	2.663663	-0.535145
H	4.067534	1.848798	-1.311413

- **E(PBE-PBE)** = -1612.21490436
- **One imaginary frequency** of -724.8153
- **Zero-point correction** = 0.375031
- **Sum of electronic and thermal Enthalpies** = -1611.807076
- **Sum of electronic and thermal Free Energies** = -1611.904676

TS-trans Cyclohexyloxynitrene species A-equatorial (Figure 4)

Rh	-0.263669	-0.174936	-0.370206
Rh	-2.283754	0.560710	0.733726
O	0.672034	1.477204	0.422412
O	-1.242500	2.152546	1.474303
O	-1.393964	-1.754986	-1.047813
O	-3.302424	-1.026765	-0.014402
O	-0.821513	0.965861	-1.999286
O	-2.740041	1.651058	-0.940574
O	0.216948	-1.229851	1.331053
O	-1.734292	-0.582289	2.349723
C	-0.008721	2.285365	1.161762
C	-1.929483	1.615687	-1.935090
C	-2.637191	-1.849335	-0.744157
C	-0.625817	-1.223953	2.305658
N	1.293600	-0.840531	-1.417330
C	1.891331	-2.031916	-1.050904
O	1.320986	-3.099824	-1.276302
O	3.156564	-2.046290	-0.501748
H	2.241587	0.118182	-1.515333
C	-0.269680	-2.082467	3.498515
H	-0.479142	-3.138788	3.256230
H	0.805713	-2.000785	3.719698

H	-0.867058	-1.791062	4.374016
C	0.727384	3.495950	1.688944
H	1.661480	3.184369	2.184207
H	1.001485	4.155454	0.847883
H	0.094587	4.050624	2.395642
C	-2.327171	2.391313	-3.171756
H	-1.434204	2.727736	-3.718822
H	-2.907657	1.730147	-3.838856
H	-2.961312	3.247281	-2.897960
C	-3.379616	-3.030787	-1.322555
H	-3.597684	-2.836242	-2.386881
H	-2.749676	-3.931914	-1.271153
H	-4.326470	-3.186542	-0.785978
C	3.689847	-0.782641	-0.065186
C	5.147573	-0.971168	0.381467
C	3.620101	0.234356	-1.177755
H	3.086422	-0.430249	0.795657
C	5.736209	0.392893	0.789889
H	5.722147	-1.404238	-0.458825
H	5.190802	-1.693910	1.215460
C	4.127557	1.601552	-0.793642
H	4.033206	-0.159217	-2.124462
C	5.604249	1.441832	-0.329028
H	6.797970	0.270638	1.069365
H	5.214337	0.759022	1.696066
H	4.063709	2.309290	-1.637858
H	3.522831	2.012710	0.034911
H	6.222498	1.136698	-1.195148
H	5.989434	2.421259	0.009141

- **E(PBE-PBE)** = -1612.21294698
- **One imaginary frequency** of -1303.6273
- **Zero-point correction**= 0.374805
- **Sum of electronic and thermal Enthalpies** = -1611.805153
- **Sum of electronic and thermal Free Energies** = -1611.904199

Cyclohexyloxynitrene species A-axial (B) (Figure 3)

Rh	0.472254	-0.168148	-0.557010
Rh	2.305968	0.408608	0.914625
O	0.993834	-2.122639	-0.213920
O	2.728699	-1.562459	1.162878
O	0.147551	1.866330	-0.715286
O	1.889737	2.382122	0.672152
O	1.801166	-0.064759	-2.134798
O	3.534159	0.470750	-0.725802
O	-0.756544	-0.240823	1.100281
O	0.989007	0.310808	2.485641
C	1.993887	-2.410253	0.541697
C	3.025196	0.239977	-1.881587
C	0.899488	2.694004	-0.080288

C	-0.229988	-0.008567	2.254089
N	-0.918628	-0.617021	-1.783851
C	-2.098282	-1.164073	-1.368440
O	-2.173193	-2.404217	-1.301477
O	-3.113197	-0.295878	-1.173902
C	2.330029	-3.875224	0.677009
H	1.407674	-4.471254	0.749749
H	2.870982	-4.205247	-0.226858
H	2.970178	-4.039196	1.555546
C	3.941676	0.365350	-3.078024
H	3.646577	-0.347552	-3.862101
H	3.851593	1.384265	-3.493710
H	4.986790	0.203020	-2.777037
C	-1.143819	-0.160034	3.449276
H	-2.163672	0.169434	3.200336
H	-1.192121	-1.227010	3.729537
H	-0.749391	0.408164	4.303929
C	0.557847	4.157912	-0.225670
H	0.300876	4.386031	-1.271476
H	-0.326749	4.386634	0.393680
H	1.399487	4.780203	0.110108
C	-4.433028	-0.898135	-0.921211
C	-5.467839	0.087707	-1.470363
C	-4.600392	-1.142232	0.585067
H	-4.465142	-1.856156	-1.467286
C	-5.513014	1.397267	-0.663481
H	-6.454591	-0.413276	-1.423553
H	-5.256717	0.285451	-2.536095
C	-4.642993	0.172861	1.381123
H	-5.548924	-1.697246	0.726513
H	-3.786542	-1.799883	0.936041
C	-5.721917	1.124374	0.836050
H	-6.315574	2.048753	-1.054315
H	-4.560979	1.941635	-0.808450
H	-4.821756	-0.043456	2.450835
H	-3.652790	0.661489	1.308913
H	-5.717919	2.074205	1.401604
H	-6.721759	0.669954	0.990749

- **E(PBE-PBE) = -1612.23834801**
- **No imaginary frequency**
- **Zero-point correction=** 0.380953
- **Sum of electronic and thermal Enthalpies=** -1611.823998
- **Sum of electronic and thermal Free Energies=** -1611.924383

TS-Cis Cyclohexyloxynitrene species A-axial (Figure 3)

Rh	0.226157	-0.059733	-0.332875
Rh	2.417763	0.276121	0.626279
O	-0.430659	1.504672	0.834911
O	1.643428	1.800686	1.748998
O	1.081884	-1.582937	-1.415282
O	3.156659	-1.240506	-0.507522
O	-0.182705	-1.372479	1.197849
O	1.912571	-1.075931	2.084900
O	0.743308	1.284372	-1.810036
O	2.820108	1.603334	-0.882148
C	0.405448	2.092840	1.621803
C	0.749785	-1.614066	2.054543
C	2.332724	-1.842432	-1.288309
C	1.912157	1.820996	-1.762855
N	-1.557032	-0.345535	-1.210351
O	-2.241180	-1.522473	-0.942331
O	-1.878831	-2.568452	-1.476249
O	-3.344828	-1.493481	-0.126623
C	-0.144822	3.205985	2.484320
H	-0.859058	3.818088	1.912076
H	-0.684912	2.770247	3.343104
H	0.674824	3.831563	2.865349
C	0.434520	-2.653898	3.106139
H	-0.583154	-2.503211	3.498943
H	0.463965	-3.654710	2.641629
H	1.171521	-2.613112	3.920458
C	2.230503	2.819508	-2.854511
H	1.944911	2.406880	-3.835041
H	1.638077	3.737037	-2.696435
H	3.299779	3.073196	-2.843594
C	2.875322	-2.948254	-2.163302
H	2.155990	-3.780310	-2.206519
H	3.005130	-2.566003	-3.190658
H	3.847957	-3.294092	-1.785293
C	-3.509506	-0.248287	0.600034
C	-4.916867	-0.243027	1.211385
C	-3.309110	0.904706	-0.366144
H	-2.741010	-0.221270	1.394095
C	-6.013351	-0.127524	0.140644
H	-4.973546	0.618255	1.905047
H	-5.044033	-1.156350	1.819207
C	-4.388109	1.038571	-1.430439
H	-3.061331	1.845229	0.153813
H	-2.289071	0.660752	-1.003478
C	-5.784159	1.094903	-0.761402
H	-7.003185	-0.063827	0.627337
H	-6.016448	-1.046003	-0.474664
H	-4.210392	1.937113	-2.045885
H	-4.353936	0.166171	-2.109503
H	-6.559381	1.153335	-1.547011
H	-5.867479	2.022802	-0.161539

- **E(UPBE-PBE)** = -1612.21804229
- **One imaginary frequency** of -21.1338
- **Zero-point correction**= 0.377491
- **Sum of electronic and thermal Enthalpies**= -1611.808147
- **Sum of electronic and thermal Free Energies**= -1611.905365

- ***4-tert-Butyl-cyclohexyloxynitrene species (Figure 5)***

Rh	1.141491	0.316166	-0.437173
Rh	2.699168	-1.067280	0.794733
O	0.757297	1.336612	1.306062
O	2.260072	0.045960	2.465555
O	1.596868	-0.792804	-2.120343
O	3.064766	-2.101393	-0.934133
O	-0.294145	-1.082190	0.083918
O	1.196866	-2.362411	1.249155
O	2.735541	1.552857	-0.794346
O	4.200487	0.222853	0.347118
C	1.408376	0.997871	2.366757
C	0.026942	-2.105904	0.796240
C	2.450674	-1.748314	-2.004913
C	3.905731	1.257868	-0.350852
N	-0.065874	1.388245	-1.469021
C	-0.512877	2.609500	-1.064049
O	0.230968	3.575516	-1.312621
O	-1.742351	2.790101	-0.539479
H	-2.600032	0.982094	-2.399382
C	5.018122	2.210259	-0.714634
H	5.317561	2.031908	-1.761998
H	4.664820	3.250074	-0.641864
H	5.887258	2.047315	-0.061585
C	1.145356	1.834612	3.597812
H	1.667468	2.801520	3.493185
H	0.069352	2.048850	3.689819
H	1.515891	1.322280	4.496778
C	-1.074592	-3.096769	1.090294
H	-2.040964	-2.581308	1.199026
H	-1.159333	-3.802230	0.245165
H	-0.836735	-3.668957	1.998749
C	2.770434	-2.513218	-3.269781
H	1.847282	-2.711165	-3.835996
H	3.426992	-1.898104	-3.909020
H	3.284827	-3.454219	-3.028597
C	-2.566711	1.597452	-0.322772
C	-3.531280	1.921006	0.814215
C	-3.321032	1.229357	-1.600283
H	-1.908616	0.760985	-0.023378
C	-4.478965	0.734926	1.068575
H	-4.113258	2.821844	0.538854
H	-2.962280	2.169310	1.728181

C	-4.266836	0.042113	-1.344303
H	-3.898460	2.112762	-1.935015
C	-5.265924	0.323994	-0.197619
H	-5.168175	1.000627	1.888250
H	-3.881886	-0.126727	1.428677
H	-4.801345	-0.191614	-2.280731
H	-3.657248	-0.850336	-1.098848
H	-5.862747	1.210691	-0.505431
C	-6.309913	-0.823616	0.044884
C	-7.075100	-1.121172	-1.264506
C	-5.645933	-2.127712	0.537336
C	-7.348892	-0.369137	1.095397
H	-7.509800	-0.199286	-1.692696
H	-6.429856	-1.581237	-2.031817
H	-7.905884	-1.823371	-1.071289
H	-5.149027	-1.993479	1.514410
H	-6.406971	-2.918565	0.664569
H	-4.896507	-2.505889	-0.180326
H	-8.144698	-1.128018	1.201912
H	-6.902642	-0.222803	2.093800
H	-7.829913	0.579980	0.795665

- **E(PBE-PBE)** = -1769.25522860
- **No imaginary frequency**
- **Zero-point correction** = 0.490943
- **Sum of electronic and thermal Enthalpies** = -1768.725224
- **Sum of electronic and thermal Free Energies** = -1768.837841

TS Cis-4-tert-Butyl-cyclohexyloxynitrene species (Figure 5)

Rh	1.033342	0.297494	-0.400359
Rh	2.657458	-1.070284	0.760363
O	0.714708	1.315884	1.358700
O	2.273920	0.034203	2.451064
O	1.427932	-0.810927	-2.100521
O	2.968033	-2.096817	-0.983491
O	-0.374408	-1.101371	0.176506
O	1.178825	-2.376512	1.263019
O	2.612641	1.542761	-0.818095
C	1.414512	0.981920	2.389967
C	-0.014355	-2.122150	0.875077
C	2.291138	-1.761589	-2.021426
C	3.801868	1.256032	-0.424743
N	-0.163809	1.398521	-1.423561
C	-0.473357	2.678673	-1.064886
O	0.343515	3.568100	-1.354960
O	-1.676749	2.969481	-0.523151
H	-2.013965	0.726400	-2.058151
C	4.890979	2.215646	-0.837085
H	5.152854	2.030760	-1.893324
H	4.530389	3.252558	-0.759805

H	5.785317	2.065748	-0.215601
C	1.201998	1.817645	3.631309
H	1.706620	2.790534	3.499985
H	0.129330	2.019212	3.776129
H	1.622183	1.311213	4.511586
C	-1.095606	-3.096935	1.279298
H	-1.179579	-3.111744	2.378987
H	-2.064060	-2.818636	0.840966
H	-0.814762	-4.112818	0.957127
C	2.502092	-2.579403	-3.275945
H	2.420352	-1.939418	-4.167117
H	3.480773	-3.079569	-3.244990
H	1.714884	-3.350938	-3.339838
C	-2.502699	1.809467	-0.202864
C	-3.743501	2.306843	0.528856
C	-2.879585	1.019696	-1.444927
H	-1.914886	1.158222	0.474625
C	-4.652249	1.119411	0.898977
H	-4.282593	3.011694	-0.132066
H	-3.447244	2.865905	1.434366
C	-3.772997	-0.172096	-1.082596
H	-3.636455	1.845981	-2.237780
C	-5.050980	0.266461	-0.328276
H	-5.547897	1.510171	1.411543
H	-4.122242	0.483539	1.635429
H	-4.027206	-0.717882	-2.006723
H	-3.181689	-0.868715	-0.455061
H	-5.605229	0.938296	-1.019371
C	-6.039904	-0.907240	0.002547
C	-6.448246	-1.627671	-1.302336
C	-5.426083	-1.943817	0.967342
C	-7.328318	-0.338865	0.640544
H	-6.837386	-0.912165	-2.049618
H	-5.606266	-2.173533	-1.760746
H	-7.244365	-2.365964	-1.098639
H	-5.150237	-1.494533	1.937261
H	-6.153161	-2.749848	1.173363
H	-4.524622	-2.418393	0.540097
H	-8.081721	-1.138096	0.758851
H	-7.149763	0.090608	1.640938
H	-7.773385	0.449227	0.005988

- **E(PBE-PBE) =** -1769.22714191

- **One imaginary frequency of** -63.0729
- **Zero-point correction =** 0.487498
- **Sum of electronic and thermal Enthalpies =** -1768.701790
- **Sum of electronic and thermal Free Energies =** -1768.810227

TS Trans-4-tert-Butyl-cyclohexyloxynitrene species (Figure 5)

Rh	1.065868	0.284733	-0.408957
Rh	2.683859	-1.051872	0.789639
O	0.713756	1.316959	1.336374
O	2.284343	0.076587	2.458971
O	1.482367	-0.845613	-2.086901
O	3.016992	-2.105667	-0.933654
O	-0.358399	-1.093922	0.143615
O	1.180355	-2.344467	1.282760
O	2.631195	1.541129	-0.846966
O	4.152900	0.253248	0.278985
C	1.412055	1.012167	2.375361
C	-0.004113	-2.103774	0.862473
C	2.358460	-1.781269	-1.987253
C	3.815280	1.268133	-0.434074
N	-0.184403	1.394633	-1.501280
C	-0.503586	2.673712	-1.079931
O	0.298819	3.600684	-1.175052
O	-1.796313	2.963796	-0.638781
H	-1.385725	0.809764	-1.593206
C	4.907808	2.222578	-0.854760
H	5.222147	1.978839	-1.884622
H	4.527396	3.255049	-0.855665
H	5.776874	2.126501	-0.188106
C	1.189004	1.869638	3.600885
H	1.715854	2.830264	3.465667
H	0.117973	2.094490	3.720624
H	1.581976	1.370136	4.497704
C	-1.096244	-3.078799	1.241623
H	-1.863230	-2.564384	1.845500
H	-1.589556	-3.460252	0.332299
H	-0.677726	-3.915864	1.817549
C	2.657983	-2.557821	-3.250848
H	1.735025	-2.715706	-3.829182
H	3.351243	-1.971904	-3.879086
H	3.131042	-3.519649	-3.006081
C	-2.640934	1.886116	-0.205705
C	-3.996529	2.435947	0.269922
C	-2.899667	0.883298	-1.304358
H	-2.147448	1.372395	0.644067
C	-4.891022	1.261227	0.712706
H	-4.467402	2.994924	-0.560145
H	-3.839336	3.147913	1.099899
C	-3.692040	-0.313659	-0.887562
H	-3.175555	1.342174	-2.268945
C	-5.094934	0.193264	-0.389592
H	-5.866328	1.665815	1.032642
H	-4.439712	0.787099	1.605930
H	-3.810715	-1.019168	-1.725575
H	-3.178611	-0.840280	-0.064149
H	-5.573574	0.701314	-1.253451
C	-6.064834	-0.976769	0.009593

C	-6.250223	-1.938686	-1.185010
C	-5.549417	-1.781084	1.221688
C	-7.453974	-0.389726	0.353598
H	-6.560859	-1.394759	-2.095712
H	-5.330231	-2.500733	-1.419426
H	-7.034927	-2.681190	-0.955959
H	-5.446674	-1.152952	2.123468
H	-6.258674	-2.591680	1.466240
H	-4.571491	-2.252657	1.018937
H	-8.177463	-1.205917	0.527582
H	-7.434655	0.229377	1.266035
H	-7.843109	0.231048	-0.473908

- **E(PBE-PBE) =** -1769.22324337
- **One imaginary frequency of** -1481.6208
- **Zero-point correction =** 0.484399
- **Sum of electronic and thermal Enthalpies =** -1768.700229
- **Sum of electronic and thermal Free Energies =** -1768.811129

4-tert-Butyl-1-methyl-cyclohexyloxynitrene species (Figure 6)

Rh	-1.265850	-0.033296	-0.201821
Rh	-3.572677	0.430571	0.364512
O	-1.404243	-1.765327	0.895376
O	-3.605189	-1.346053	1.392414
O	-1.236822	1.755372	-1.243374
O	-3.427285	2.179000	-0.696927
O	-0.766161	0.968718	1.523086
O	-2.947579	1.389233	2.045185
O	-2.044292	-0.983232	-1.857056
O	-4.214382	-0.528244	-1.300410
C	-2.536211	-2.052823	1.438472
C	-1.689572	1.468635	2.269280
C	-2.313524	2.458992	-1.270792
C	-3.311126	-1.039922	-2.056391
N	0.501771	-0.425688	-0.838310
C	1.048098	-1.667150	-0.793514
O	0.535253	-2.568644	-1.481456
O	2.182219	-1.924201	-0.093148
H	2.760087	0.530237	-1.335522
C	-3.758025	-1.772391	-3.298360
H	-3.375679	-1.250564	-4.191403
H	-3.328705	-2.787245	-3.302793
H	-4.855174	-1.822307	-3.337745
C	-2.598511	-3.368043	2.180576
H	-2.625991	-4.193118	1.448127
H	-1.692981	-3.500506	2.792732
H	-3.499290	-3.412096	2.808754
C	-1.230882	2.219111	3.496193
H	-0.478386	1.628268	4.042006

H	-0.751583	3.164188	3.188212
H	-2.087117	2.442450	4.147886
C	-2.260628	3.730223	-2.088934
H	-1.258877	4.181366	-2.030302
H	-2.459985	3.485090	-3.146806
H	-3.027197	4.439163	-1.744191
C	3.166307	-0.877186	0.273242
C	4.355522	-1.708342	0.793262
C	3.590565	-0.111759	-0.993248
C	5.634641	-0.875377	0.987968
H	4.548117	-2.507435	0.053489
H	4.067911	-2.209229	1.735700
C	4.869999	0.719086	-0.788660
H	3.770605	-0.860020	-1.789119
C	6.054168	-0.149390	-0.309345
H	6.434622	-1.551683	1.335297
H	5.482410	-0.135655	1.797950
H	5.109434	1.217037	-1.743994
H	4.678752	1.528154	-0.057235
H	6.205517	-0.936255	-1.081150
C	7.422954	0.613168	-0.214295
C	7.783288	1.209860	-1.593545
C	7.390292	1.751561	0.827174
C	8.544969	-0.378510	0.169123
H	7.770213	0.433811	-2.380901
H	7.090772	2.013060	-1.897461
H	8.798525	1.644910	-1.569712
H	7.176805	1.374552	1.842775
H	8.369701	2.261692	0.865188
H	6.631900	2.514967	0.579997
H	9.529343	0.121226	0.126121
H	8.424343	-0.773560	1.192187
H	8.575904	-1.237651	-0.526135
C	2.571879	0.021367	1.361009
H	1.730146	0.615262	0.966257
H	2.197730	-0.592180	2.198154
H	3.332060	0.716896	1.755878

- **E(PBE-PBE) =** -1808.50659332
- **No imaginary frequency**
- **Zero-point correction=** 0.517176
- **Sum of electronic and thermal Enthalpies=** -1807.948804
- **Sum of electronic and thermal Free Energies=** -1808.064401

TS Cis-4-tert-Butyl-1-methyllcyclohexyloxynitrene species (Figure 6)

Rh	1.122931	0.185439	-0.271546
Rh	3.159515	-0.857451	0.521184
O	1.238733	1.490292	1.311045
O	3.194831	0.528801	2.033952
O	1.111697	-1.187059	-1.819347
O	3.023643	-2.188863	-1.031609
O	0.121056	-1.163717	0.914533
O	2.048209	-2.105688	1.685463
O	2.374886	1.405690	-1.358392
O	4.281006	0.374876	-0.630766
C	2.251415	1.394421	2.103297
C	0.774092	-2.007827	1.636042
C	2.053069	-2.063389	-1.863371
C	3.648549	1.251174	-1.324751
N	-0.399622	1.068861	-1.053080
C	-0.775467	2.362634	-0.862904
O	0.006168	3.248810	-1.257657
O	-2.010332	2.695377	-0.416962
H	-2.163624	0.278143	-1.626333
C	4.455998	2.176263	-2.202642
H	4.385310	1.834791	-3.249841
H	4.041621	3.194876	-2.156033
H	5.511015	2.169996	-1.893770
C	2.325908	2.424126	3.207339
H	2.551570	3.410340	2.766891
H	1.351304	2.505833	3.714056
H	3.111304	2.157850	3.928333
C	-0.035541	-2.956197	2.487618
H	-1.111551	-2.766541	2.372399
H	0.193237	-3.994901	2.196908
H	0.254595	-2.838400	3.544684
C	2.016345	-3.021492	-3.033176
H	0.982436	-3.346456	-3.226035
H	2.375748	-2.500101	-3.937297
H	2.664603	-3.888016	-2.840405
C	-2.926571	1.614003	-0.022018
C	-4.283881	2.284225	0.245295
C	-3.104241	0.635978	-1.183670
C	-5.379301	1.239719	0.559230
H	-4.556771	2.869418	-0.651604
H	-4.193357	2.997903	1.084741
C	-4.075871	-0.488528	-0.800476
H	-3.811513	1.286295	-2.164011
C	-5.478158	0.085133	-0.470087
H	-6.345354	1.770242	0.618178
H	-5.203912	0.825490	1.569818
H	-4.147233	-1.197574	-1.642687
H	-3.671845	-1.061096	0.056502
H	-5.842328	0.540176	-1.417334
C	-6.543011	-1.006458	-0.088735
C	-6.704225	-2.002987	-1.258757

C	-6.152497	-1.796245	1.179289
C	-7.915838	-0.337788	0.149208
H	-5.789331	-2.594278	-1.433047
H	-7.520129	-2.716548	-1.044836
H	-6.955592	-1.479044	-2.199038
H	-6.042308	-1.140539	2.060834
H	-6.935350	-2.537924	1.419954
H	-5.206776	-2.349922	1.045632
H	-8.697795	-1.106347	0.285225
H	-7.920570	0.297102	1.051443
H	-8.210302	0.290355	-0.711572
C	-2.381884	0.976728	1.269481
H	-1.512797	0.329996	1.084877
H	-2.079554	1.781325	1.961209
H	-3.149940	0.366985	1.770637

- E(PBE-PBE) = -1808.47460662
- One imaginary frequency of -75.0930
- Zero-point correction = 0.514351
- Sum of electronic and thermal Enthalpies = -1807.920975
- Sum of electronic and thermal Free Energies = -1808.032740

TS trans-4-tert-Butyl-1-methyllcyclohexyloxynitrene species (Figure 6)

Rh	-1.096948	0.275241	-0.254161
Rh	-2.970035	-1.069842	0.467407
O	-1.281280	-0.608593	-2.115151
O	-3.072729	-1.865454	-1.415425
O	-0.996444	1.057578	1.640553
O	-2.787644	-0.203921	2.320248
O	0.142623	-1.252962	0.337028
O	-1.636103	-2.525514	1.004091
O	-2.483619	1.689267	-0.791514
O	-4.248917	0.409865	-0.086383
C	-2.222964	-1.465630	-2.291960
C	-0.384587	-2.318457	0.836959
C	-1.866069	0.668205	2.506417
C	-3.733441	1.468815	-0.602643
N	0.446509	1.399808	-0.898993
C	0.655639	2.674367	-0.368377
O	-0.155916	3.589279	-0.375945
O	1.952956	2.933252	0.173975
H	1.470758	1.030535	-0.484307
C	-4.680512	2.555165	-1.057110
H	-4.250876	3.544270	-0.837537
H	-4.816251	2.483081	-2.150302
H	-5.659235	2.438200	-0.570003
C	-2.357595	-2.036259	-3.687451
H	-2.966353	-1.348404	-4.300131
H	-1.368789	-2.125088	-4.161722
H	-2.862151	-3.012881	-3.655859
C	0.567899	-3.400615	1.294563

H	1.478843	-3.403903	0.676861
H	0.861893	-3.207439	2.341368
H	0.074127	-4.382439	1.252943
C	-1.804360	1.332945	3.863323
H	-0.762112	1.561021	4.132582
H	-2.356411	2.288032	3.818716
H	-2.272339	0.693114	4.625423
C	3.042985	2.072544	-0.254247
C	4.275586	2.272743	0.653832
C	2.622404	0.615397	-0.018177
C	5.353925	1.212592	0.328791
H	3.949286	2.187773	1.706444
H	4.683594	3.291574	0.517911
C	3.548905	-0.432425	-0.517878
H	2.265732	0.448706	1.012556
C	4.854441	-0.257778	0.356148
H	6.174357	1.328204	1.057430
H	5.793126	1.437071	-0.660224
H	3.127245	-1.437731	-0.364591
H	3.779178	-0.309197	-1.589485
H	4.545208	-0.473896	1.400863
C	5.962373	-1.319746	0.013429
C	5.383533	-2.744527	0.161134
C	6.517921	-1.152622	-1.416052
C	7.125755	-1.178467	1.023026
H	4.906744	-2.884525	1.148857
H	4.636364	-2.975967	-0.617122
H	6.189145	-3.494207	0.070581
H	7.001577	-0.171361	-1.561567
H	7.281142	-1.925392	-1.616534
H	5.731822	-1.264245	-2.183065
H	7.859445	-1.990123	0.872094
H	7.665947	-0.223918	0.907644
H	6.763645	-1.244254	2.065283
C	3.346764	2.402990	-1.725544
H	2.482151	2.152683	-2.361923
H	3.539365	3.485273	-1.805549
H	4.227446	1.866022	-2.111668

- **E(UPBE-PBE) =** -1808.47123733
- **One imaginary frequency of** -145.6071
- **Zero-point correction =** 0.513277
- **Thermal correction to Energy=** 0.551907
- **Sum of electronic and thermal Enthalpies =** -1807.918386
- **Sum of electronic and thermal Free Energies =** -1808.030094