Electronic Supplementary Information

for

$S_8$-Promoted Triple Cleavage of Bromodifluoro Compounds for the Assembly of $N$-containing Heterocycles

Shuilin Deng$^1$, Haohua Chen$^1$, Xingxing Ma$^1$, Yao Zhou$^1$, Kai Yang$^2$, Yu Lan$^{4,5,*}$ and Qiuling Song$^{1,2,3,*}$

$^1$ Institute of Next Generation Matter Transformation, College of Chemical Engineering and College of Material Sciences Engineering at Huaqiao University, 668 Jimei Boulevard, Xiamen, Fujian, China, 361021

$^2$ College of Chemistry, Fuzhou University, Fuzhou, Fujian, China, 350108

$^3$ State Key Laboratroy of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, P. R. China

$^4$ School of Chemistry and Chemical Engineering, Chongqing University, Chongqing 400030, P. R. China

$^5$ College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou 450001, P. R. China.
Table of Contents

1. General information .................................................................................................1

2. General procedure for starting materials ...............................................................2

3. General process for the synthesis of 2-carbonylbenzoxazole .................................2

4. Control experiments ................................................................................................4

5. Crystal Structure ....................................................................................................4

6. Computation ............................................................................................................9

7. Characterization data for products .........................................................................12

8. References ..............................................................................................................33

9. NMR spectroscopic data .......................................................................................34
1. General information

All chemicals were purchased from Adamas Reagent, energy chemical company, J&K Scientific Ltd, Bide Pharmatech Ltd and Tansoole. Unless stated otherwise, reactions were performed in oven-dried or flame-dried glassware using a Schlenkline under a nitrogen atmosphere. All solvents were commercially obtained, and reactions were performed without specific drying of solvents. Flash column chromatography was performed over silica gel (200-300 mesh). $^1$H-NMR and $^{13}$C-NMR spectra were recorded in CDCl$_3$ on a Bruker Avance 500 spectrometer (500 MHz $^1$H, 125 MHz $^{13}$C) at room temperature. Chemical shifts were reported in ppm on the scale relative to CDCl$_3$ ($\delta = 7.26$ for $^1$H-NMR, $\delta = 77.00$ for $^{13}$C-NMR) as an internal reference. Coupling constants ($J$) were reported in Hertz (Hz). The following abbreviations are used to indicate signal multiplicity: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, and br = broad. High resolution mass spectra were recorded using a Thermo Fisher Scientific LTQ FT Ultra or Waters Micromass GCT Premier instrument.
2. General procedure for starting materials

General procedure for the synthesis of bromodifluoroacetamides

\[
RR'NH + \text{BrCF}_2\text{CO}_2\text{Et} \xrightarrow{\text{La(OTf)}_3, \text{rt}} \text{BrCF}_2\text{CONRR'}
\]

To a round-bottom flask equipped with stir bar was added amine (5 mmol) under argon, then ethyl bromodifluoroacetate (1.2 equiv) was added with lanthanum trifluoromethanesulfonate (5 mol %). The mixture was stirred at the room temperature and monitored by TLC. After the amine was exhausted, the mixture was extracted with AcOEt, and then the extract was washed with brine and dried over MgSO₄. The solvent was removed in vacuo and the residue was purified by column chromatography on silica gel to give the corresponding amide 2.

3. General process for the synthesis of 2-carbonylbenzoxazole

General process for the synthesis of 2-carbonylbenzimidazole (1)

\[
\begin{align*}
\text{NH}_2
& \quad \text{BrCF}_2\text{COR} \\
\text{NH}_2
\end{align*}
\xrightarrow{\text{S}_8, \text{Na}_2\text{CO}_3, \text{solvent}} \quad \begin{align*}
\text{N} \\
\text{R}
\end{align*}
\]

To a mixture of O-phenylenediamine 1 (0.3 mmol, 1.0 equiv), S₈ (15.39 mg, 20 mol %) and Na₂CO₃ (95.4 mg, 3 equiv) with BrCF₂COR (1.2 equiv) was added MeCN (1 mL). The resulting mixture was heated to 130 °C. After 16 h, the mixture was cooled to room temperature. Upon completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography to give the desired product 3.
General process for the synthesis of 2-carbonylbenzoxazole (2)

To a mixture of O-aminophenol 1 (0.3 mmol, 1.0 equiv), S₈ (15.39 mg, 20 mol %) and Na₂CO₃ (95.4 mg, 3 equiv) with BrCF₂COR (1.2 equiv) was added MeCN (2 mL). The resulting mixture was heated to 120 °C. After 12 h, the mixture was cooled to room temperature. Upon completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography to give the desired product 3.

General process for the synthesis of 2-carbonylbenzothiazole (3)

To a mixture of O-aminothiophenol 1 (0.2 mmol, 1.0 equiv), S₈ (5.12 mg, 10 mol %) and Na₂CO₃ (63.6 mg, 3 equiv) with BrCF₂COR (1.2 equiv) was added MeCN (2 mL). The resulting mixture was heated to 90 °C. After 12 h, the mixture was cooled to room temperature. Upon completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography to give the desired product 3.
4. Control experiments

a. 

\[
\text{7} \quad \text{NH}_2 + \text{Br}_2 \text{CO} \quad \xrightarrow{\text{Na}_2\text{CO}_3 (3 \text{ equiv})} \quad \xrightarrow{\text{MeCN (2 mL), 130 °C, N}_2} \quad \text{8} \quad \text{NH}_2
\]

\[
\text{69%}
\]

b. 

\[
\text{4} \quad \text{NH}_2 + \text{Br}_2 \text{CO} \quad \xrightarrow{\text{Na}_2\text{CO}_3 (3 \text{ equiv})} \quad \xrightarrow{\text{MeCN (2 mL), 120 °C, N}_2} \quad \text{5} \quad \text{NH}_2 \quad \xrightarrow{\text{50%}} \quad \text{6} \quad \text{NH}_2 \quad \xrightarrow{\text{40%}}
\]

5. Crystal Structure

Crystal Structure of 5h (1)

Crystallographic data for compound 5h (CCDC-1883275) has been deposited with the Cambridge Crystallographic Data Centre, Copies of the data can be obtained, free of charge, on application to CCDC (Email: deposit@ccdc.cam.ac.uk).
Crystal Structure of 7h (2)

Crystallographic data for compound 7h (CCDC-1883277) has been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained, free of charge, on application to CCDC (Email: deposit@ccdc.cam.ac.uk).
Bond precision:  C-C = 0.0041 Å  Wavelength=0.71073

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Data completeness= 0.997  Theta(max)= 25.000
R(reflections)= 0.0471(1874)  wR2(reflections)= 0.1584(2586)
S = 0.998  Npar= 181
Crystal Structure of S4-c7 (3)

Crystallographic data for compound S4-c7 (CCDC-1875544) has been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained, free of charge, on application to CCDC (Email: deposit@ccdc.cam.ac.uk).
Bond precision:  C-C = 0.0057 Å  
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Data completeness = 0.997  
θ(max) = 24.994

R(reflections) = 0.0894 (1154)  
wr2(reflections) = 0.2188 (1461)

S = 1.396  
Npar = 118
6. Computation

Complete Reference for Gaussian 09 (1)


Computational Methods (2)

All the DFT calculations were carried out with the GAUSSIAN 09 series of programs. DFT method B3-LYP\(^2\) with a standard 6–31G(d) basis set was used for geometry optimizations. Harmonic vibrational frequency calculations were performed for all of the stationary points to confirm them as a local minima or transition structures, and to derive the thermochemical corrections for the enthalpies and free energies. The M11\(^3\) functional in combination with the 6–311+G(d,p) basis set was used to calculate the solvation single point energies to give more accurate energy information. The solvent effects were considered by single point calculations on the gas-phase stationary points with an SMD\(^4\) solvation model in the acetonitrile solvent.
Absolute Calculation Energies, Enthalpies, and Free Energies (3)

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$^1$The electronic energy calculated by B3LYP in gas phase. $^2$The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. $^3$The thermal correction to enthalpy calculated by B3LYP in gas phase. $^4$The electronic energy calculated by M11 in diethylether solvent. $^5$The B3LYP calculated imaginary frequencies for the transition states.

B3LYP Geometries for All the Optimized Compounds and Transition State (4)

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TS
7. Characterization data for products

**N-isopropyl-1H-benzo[d]imidazole-2-carboxamide (3a) (CAS Number: 214962-82-0)**

Compound 3a was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 89% yield (54 mg).

$^1$H NMR (500 MHz, DMSO) $\delta$ 13.24 (s, 1H), 8.71 (d, $J = 8.5$ Hz, 1H), 7.71 (d, $J = 6.2$ Hz, 1H), 7.54 (d, $J = 6.3$ Hz, 1H), 7.34 – 7.20 (m, 2H), 4.28 – 4.03 (m, 1H), 1.20 (t, $J = 8.8$ Hz, 6H). $^{13}$C NMR (125 MHz, DMSO) $\delta$ 158.3, 146.4, 143.0, 134.9, 124.4, 122.8 (d, $J = 21.2$ Hz), 120.2, 113.0, 109.9, 41.3, 22.5.

**N-(tert-butyl)-1H-benzo[d]imidazole-2-carboxamide (3b) (CAS Number: 306992-74-5)**

Compound 3b was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 93% yield (59 mg).

$^1$H NMR (500 MHz, DMSO) $\delta$ 13.21 (s, 1H), 7.95 (s, 1H), 7.71 (d, $J = 6.1$ Hz, 1H), 7.53 (d, $J = 6.1$ Hz, 1H), 7.28 (d, $J = 6.8$ Hz, 2H), 1.43 (s, 9H). $^{13}$C NMR (125 MHz, DMSO) $\delta$ 158.6, 146.7, 142.8, 135.0, 124.5, 123.0, 120.3, 113.0, 51.5, 28.9.

**N-benzyl-1H-benzo[d]imidazole-2-carboxamide (3c) (CAS Number: 82755-99-5)**

Compound 3c was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 55% yield (41 mg).

$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 12.93 (s, 1H), 8.70 (t, $J = 5.5$ Hz, 1H), 7.76 (d, $J = 5.2$ Hz, 1H), 7.43 – 7.27 (m, 8H), 4.73 (d, $J = 6.1$ Hz, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$)
δ 159.8, 145.0, 142.7, 137.4, 134.5, 129.1, 128.8, 128.0 – 127.6, 125.0, 123.4, 120.3, 112.8, 43.8.

N-allyl-1H-benzo[d]imidazole-2-carboxamide (3d) (CAS Number: 82755-98-4)

Compound 3d was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 75% yield (45 mg). ^1H NMR (500 MHz, DMSO) δ 13.29 (s, 1H), 9.15 (t, J = 6.0 Hz, 1H), 7.78 – 7.49 (m, 2H), 7.28 (s, 2H), 5.96 – 5.85 (m, 1H), 5.19 – 5.14 (m, 1H), 5.10 – 5.06 (m, 1H), 3.94 (t, J = 5.6 Hz, 2H). ^13C NMR (125 MHz, DMSO) δ 159.1, 146.1, 135.3, 123.8, 122.9 – 121.9, 120.3, 115.8, 113.1, 41.6.

N-phenyl-1H-benzo[d]imidazole-2-carboxamide (3e) (CAS Number: 13745-42-1)

Compound 3e was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 68% yield (48 mg). ^1H NMR (500 MHz, DMSO) δ 13.49 (s, 1H), 10.92 (s, 1H), 7.96 (d, J = 7.7 Hz, 2H), 7.81 (d, J = 7.5 Hz, 1H), 7.60 (d, J = 7.5 Hz, 1H), 7.43 – 7.33 (m, 3H), 7.32 (d, J = 7.6 Hz, 1H), 7.13 (t, J = 7.4 Hz, 1H). ^13C NMR (125 MHz, DMSO) δ 157.8, 146.1, 143.0, 138.7, 135.2, 129.2, 124.9, 124.6, 123.2, 121.0, 120.5, 113.1.

N-cyclopropyl-1H-benzo[d]imidazole-2-carboxamide (3f) (CAS Number: 1531657-68-7)

Compound 3f was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 32% yield (19 mg). ^1H NMR (500 MHz, DMSO) δ 13.23 (s, 1H), 9.00 (d, J = 4.9 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.52 (d, J = 7.9 Hz, 1H), 7.34 – 7.22 (m, 2H), 3.06 – 2.80 (m,
1H), 0.76 – 0.64 (m, 4H). $^{13}$C NMR (125 MHz, DMSO) δ 160.4, 146.1, 143.0, 134.9, 124.5, 122.9, 120.2, 113.0, 23.3, 6.1.

(1H-benzo[d]imidazol-2-yl)(pyrrolidin-1-yl)methanone (3g) (CAS Number: 73902-99-5)

Compound 3g was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 74% yield (48 mg). $^1$H NMR (500 MHz, DMSO) δ 13.10 (s, 1H), 7.75 (d, $J = 8.1$ Hz, 1H), 7.53 (d, $J = 8.0$ Hz, 1H), 7.35 – 7.19 (m, 2H), 4.14 (t, $J = 6.8$ Hz, 2H), 3.57 (t, $J = 6.9$ Hz, 2H), 2.00 – 1.79 (m, 4H). $^{13}$C NMR (125 MHz, DMSO) δ 158.1, 146.7, 143.4 (s), 134., 124.6, 122.7, 120.8, 112.7, 49.3, 47.5, 26.6, 23.7.

N,N-diethyl-1H-benzo[d]imidazole-2-carboxamide (3h) (CAS Number: 30183-06-3)

Compound 3h was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 45% yield (29 mg). $^1$H NMR (500 MHz, DMSO) δ 13.08 (s, 1H), 7.73 (d, $J = 8.1$ Hz, 1H), 7.52 (d, $J = 8.0$ Hz, 1H), 7.36 – 7.11 (m, 2H), 4.08 (q, $J = 7.0$ Hz, 2H), 3.50 (q, $J = 7.1$ Hz, 2H), 1.27 – 1.20 (m, 3H), 1.17 (t, $J = 7.1$ Hz, 3H). $^{13}$C NMR (125 MHz, DMSO) δ 159.5, 146.4, 143.1, 133.8, 124.5, 122.75, 120.7, 112.6, 43.0, 41.3, 15.1, 13.2.

N,N-dibenzyl-1H-benzo[d]imidazole-2-carboxamide (3i) (CAS Number: 1222279-35-7)

Compound 3i was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 91% yield (93 mg). $^1$H NMR (500 MHz, DMSO) δ 13.37 (s, 1H), 7.71 (d, $J = 8.1$ Hz, 1H), 7.59 (d, $J = 8.1$ Hz, 1H), 7.37 – 7.22 (m, 12H), 5.53 (s, 2H), 4.61 (s, 2H). $^{13}$C NMR (125 MHz, DMSO) δ 160.4, 145.9, 142.9, 137.7, 137.2, 134.0, 129.1 (d, $J = 8.6$ Hz), 128.1 (d, $J = 18.5$ Hz), 127.8, 124.9, 123.0, 120.8, 112.8, 51.1, 48.7.
N-isopropyl-5-methyl-1H-benzo[d]imidazole-2-carboxamide (3j)

Compound 3j was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 64% yield (42 mg). $^1$H NMR (500 MHz, DMSO) $\delta$ 13.20 (d, $J$ = 54.6 Hz, 1H), 8.74 – 8.37 (m, 1H), 7.57 – 7.28 (m, 1H), 7.20 – 7.01 (m, 2H), 4.26 – 4.11 (m, 1H), 2.56 (d, $J$ = 25.2 Hz, 3H), 1.21 (d, $J$ = 6.4 Hz, 6H). $^{13}$C NMR (125 MHz, DMSO) $\delta$ 158.4, 146.4, 145.6, 142.6, 134.5, 130.1, 124.8, 124.4, 123.2, 123., 117.5, 110.3, 41.3, 22.6, 17.5, 17.2. HRMS (ESI, m/z) calcd for C$_{12}$H$_{15}$N$_3$O[M+H]$^+$: 218.1288; found: 218.1289.

N-isopropyl-5,6-dimethyl-1H-benzo[d]imidazole-2-carboxamide (3k)

Compound 3k was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 77% yield (53 mg). $^1$H NMR (500 MHz, DMSO) $\delta$ 12.97 (s, 1H), 8.60 (d, $J$ = 8.4 Hz, 1H), 7.37 (d, $J$ = 82.8 Hz, 2H), 4.19 – 4.08 (m, 1H), 2.31 (s, 6H), 1.19 (d, $J$ = 6.6 Hz, 6H). $^{13}$C NMR (125 MHz, DMSO) $\delta$ 158.4, 146.4, 145.6, 142.6, 134.5, 130.1, 124.8, 124.4, 123.2, 123., 117.5, 110.3, 41.3, 22.5, 20.5. HRMS (ESI, m/z) calcd for C$_{13}$H$_{17}$N$_3$O[M+H]$^+$: 232.1444; found: 232.1445.

5-chloro-N-isopropyl-1H-benzo[d]imidazole-2-carboxamide (3l)

Compound 3l was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 68% yield (49 mg). $^1$H NMR (500 MHz, DMSO) $\delta$ 13.40 (d, $J$ = 35.3 Hz, 1H), 8.84 – 8.68 (m, 1H), 7.79 – 7.60 (m, 1H), 7.53 (d, $J$ = 8.3 Hz, 1H), 7.36 – 7.22 (m, 1H), 4.20 – 4.09 (m, 1H), 1.20 (d, $J$ = 6.6 Hz, 6H). $^{13}$C NMR (125 MHz, DMSO) $\delta$ 157.9, 147.7, 147.4, 143.8, 141.7, 135.5, 133.7, 128.8, 127.3, 124.7, 123.5, 121.7, 119.5), 114.4, 112.6, 41.4, 22.5. HRMS (ESI, m/z) calcd for C$_{11}$H$_{12}$ClN$_3$O[M+H]$^+$: 238.0742; found: 238.0741.
N-isopropyl-5-nitro-1H-benzo[\textit{d}]imidazole-2-carboxamide (3m)

Compound 3m was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 57% yield (42 mg). $^1$H NMR (500 MHz, DMSO) $\delta$ 13.88 (s, 1H), 8.92 (d, $J = 8.3$ Hz, 1H), 8.44 (d, $J = 88.8$ Hz, 1H), 8.17 (s, 1H), 7.95 – 7.59 (m, 1H), 4.22 – 4.09 (m, 1H), 1.20 (d, $J = 6.6$ Hz, 1H). $^{13}$C NMR (125 MHz, DMSO) $\delta$ 157.4, 119.8, 116.6, 113.6, 109.7, 41.6, 22.4. HRMS (ESI, m/z) calcd for C$_{11}$H$_{12}$FN$_3$O$^\text{[M+H]}^+$: 249.0982; found: 249.0980.

N-isopropyl-5-(trifluoromethyl)-1H-benzo[\textit{d}]imidazole-2-carboxamide (3n)

Compound 3n was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 30% yield (24 mg). $^1$H NMR (500 MHz, DMSO) $\delta$ 8.87 (d, $J = 8.4$ Hz, 1H), 7.88 (d, $J = 77.4$ Hz, 2H), 7.63 – 7.57 (m, 1H), 4.21 – 4.13 (m, 1H), 1.21 (d, $J = 6.6$ Hz, 2H). $^{13}$C NMR (125 MHz, DMSO) $\delta$ 157.7, 148.8, 128.5, 126.3, 124.2, 122.0, 120.4 (s), 41.5, 22.5. $^{19}$F NMR (471 MHz, DMSO) $\delta$ -59.19 (s). HRMS (ESI, m/z) calcd for C$_{12}$H$_{12}$F$_3$N$_3$O$^\text{[M+H]}^+$: 272.1005; found: 272.1006.

ethyl 1H-benzo[\textit{d}]imidazole-2-carboxylate (3o) (CAS Number: 1865-09-4)

Compound 3o was prepared according to the general procedure (petroleum ether/ethyl acetate = 5:1 v/v). The product was obtained as a yellow solid in 47% yield (27 mg). $^1$H NMR (500 MHz, DMSO) $\delta$ 13.48 (s, 1H), 7.77 (d, $J = 8.1$ Hz, 1H), 7.57 (d, $J = 8.1$ Hz, 1H), 7.37 (t, $J = 7.5$ Hz, 1H), 7.29 (t, $J = 7.6$ Hz, 1H), 4.45 – 4.37 (m, 2H), 1.36 (t, $J = 7.1$ Hz, 3H). $^{13}$C NMR (125 MHz, DMSO) $\delta$ 159.8, 143.3, 142.2, 134.7, 125.5, 123.4, 121.2, 113.1, 62.1, 14.6.
N-phenylbenzo[d]oxazole-2-carboxamide (5a) (CAS Number: 27411-63-8)

Compound 5a was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 73% yield (52 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 9.13 (s, 1H), 7.80 (d, $J$ = 7.9 Hz, 1H), 7.78 – 7.69 (m, 2H), 7.69 – 7.57 (m, 1H), 7.52 – 7.46 (m, 1H), 7.46 – 7.34 (m, 3H), 7.23 – 7.06 (m, 1H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 155.6, 153.26, 151.46, 140.06, 136.86, 129.3, 127.6, 125.6, 125.3, 121.3, 112.0, 112.0.

N-(4-methoxyphenyl)benzo[d]oxazole-2-carboxamide (5b) (CAS Number: 56735-19-4)

Compound 5b was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 68% yield (55 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 9.08 (s, 1H), 7.81 – 7.73 (m, 1H), 7.70 – 7.57 (m, 3H), 7.49 – 7.38 (m, 2H), 6.94 – 6.86 (m, 2H), 3.79 (s, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 157.1, 155.7, 153.0, 151.3, 140.1, 130.0, 127.5, 125.7, 121.6, 121.2, 114.4, 111.9, 55.5.

N-(p-tolyl)benzo[d]oxazole-2-carboxamide (5c) (CAS Number: 921782-65-2)

Compound 5c was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 61% yield (46 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 9.07 (s, 1H), 7.85 – 7.75 (m, 1H), 7.74 – 7.64 (m, 1H), 7.64 – 7.55 (m, 2H), 7.51 – 7.41 (m, 2H), 7.19 (d, $J$ = 8.2 Hz, 2H), 2.34 (s, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 155.7, 153.1, 151.4, 140.1, 135.1, 134.3, 129.8, 127.6, 125.7, 121.2, 119.9, 112.0, 21.0.
N-(4-fluorophenyl)benzo[d]oxazole-2-carboxamide (5d) (CAS Number: 921505-14-8)

Compound 5d was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 70% yield (54 mg). $^1$H NMR (500 MHz, CDCl$_3$) δ 9.14 (s, 1H), 7.80 (t, $J = 8.7$ Hz, 1H), 7.75 – 7.69 (m, 2H), 7.66 (d, $J = 8.1$ Hz, 1H), 7.52 – 7.42 (m, 2H), 7.11 – 7.03 (m, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 160.9, 158.9, 155.4, 153.2, 151.4, 140.0, 132.8, 127.7, 125.8, 121.7, 121.3, 116.1, 115.9, 112.0. $^{19}$F NMR (471 MHz, CDCl$_3$) δ -116.2 – -116.3.

N-(4-chlorophenyl)benzo[d]oxazole-2-carboxamide (5e) (CAS Number: 27411-66-1)

Compound 5e was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 72% yield (59 mg). $^1$H NMR (500 MHz, CDCl$_3$) δ 9.16 (s, 1H), 7.79 – 7.72 (m, 1H), 7.72 – 7.66 (m, 2H), 7.65 – 7.53 (m, 1H), 7.50 – 7.45 (m, 1H), 7.45 – 7.39 (m, 1H), 7.36 – 7.28 (m, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 155.3, 153.2, 151.4 139.9, 135.4, 130.4, 129.3, 127.8, 125.8, 121.2, 111.9.

N-(2-methylbenzyl)benzo[d]oxazole-2-carboxamide (5f)

Compound 5f was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 60% yield (48 mg). $^1$H NMR (500 MHz, CDCl$_3$) δ 7.75 (d, $J = 8.0$ Hz, 1H), 7.66 (d, $J = 8.2$ Hz, 1H), 7.50 – 7.38 (m, 3H), 7.32 (d, $J = 7.2$ Hz, 1H), 7.26 – 7.13 (m, 3H), 4.69 (d, $J = 5.7$ Hz, 2H), 2.39 (s, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 155.4(d, $J = 7.0$ Hz), 151.2, 140.1, 136.6, 134.6, 130.7, 128.9, 128.3, 127.4, 126.4, 125.6, 121.2, 111.9, 42.1, 19.1. HRMS (ESI, m/z) caleed for C$_{16}$H$_{15}$N$_2$O$_2$[M+H]$^+$: 267.1128; found: 267.1126.
**N-(3-methylbenzyl)benzo[d]oxazole-2-carboxamide (5g)**

Compound 5g was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 64% yield (51 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta 7.75 (d, J = 8.0\) Hz, 1H), 7.66 (d, \(J = 8.2\) Hz, 1H), 7.51 – 7.38 (m, 3H), 7.32 (d, \(J = 7.2\) Hz, 1H), 7.26 – 7.18 (m, 3H), 4.69 (d, \(J = 5.7\) Hz, 2H), 2.39 (s, 3H). \(^1\)C NMR (125 MHz, CDCl\(_3\)) \(\delta 155.5 (d, J = 12.6\) Hz), 151.2, 140.1, 138.7, 136.9, 128.7 (d, \(J = 11.6\) Hz), 127.4, 125.6, 125.1, 121.21, 111.8, 43.90, 21.4. HRMS (ESI, m/z) calcd for C\(_{16}\)H\(_{15}\)N\(_2\)O\(_2\)[M+H]\(^+\): 267.1128; found: 267.1132.

**N-(4-methoxybenzyl)benzo[d]oxazole-2-carboxamide (5h)**

Compound 5h was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 70% yield (59 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta 7.78 – 7.68 (m, 1H), 7.67 – 7.60 (m, 2H), 7.48 – 7.42 (m, 1H), 7.42 – 7.35 (m, 1H), 7.27 (d, \(J = 8.6\) Hz, 2H), 6.86 (d, \(J = 8.6\) Hz, 2H), 4.61 (d, \(J = 5.9\) Hz, 2H), 3.78 (s, 3H). \(^1\)C NMR (125 MHz, CDCl\(_3\)) \(\delta 159.3, 155.5, 151.1, 140.1, 129.4, 129.1, 127.4, 125., 121.2, 114.2, 111.8, 55.3, 43.4. HRMS (ESI, m/z) calcd for C\(_{16}\)H\(_{14}\)N\(_2\)O\(_3\)[M+H]\(^+\): 283.1077; found: 283.1078.

**N-benzylbenzo[d]oxazole-2-carboxamide (5i) (CAS Number: 27383-78-4)**

Compound 5i was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 61% yield (49 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta 7.79 – 7.70 (m, 1H), 7.68 – 7.59 (m, 2H), 7.50 – 7.45 (m, 1H), 7.44 – 7.39 (m, 1H), 7.37 (s, 1H), 7.37 – 7.34 (m, 2H), 4.69 (d, \(J = 6.0\) Hz, 2H). \(^1\)C NMR (125 MHz, CDCl\(_3\)) \(\delta 155.6, 155.4, 151.2, 140.1, 137.0, 128.9, 128.0, 127.4, 125.6, 121.2, 111.9, 77.3, 77.1, 76.8, 43.9, 29.7.
**N-(2-fluorobenzyl)benzo[d]oxazole-2-carboxamide (5j)**

Compound 5j was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 62% yield (50 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.76 (d, $J = 7.8$ Hz, 1H), 7.69 (s, 1H), 7.64 (d, $J = 8.2$ Hz, 1H), 7.49 – 7.44 (m, 1H), 7.44 – 7.37 (m, 2H), 7.32 – 7.26 (m, 1H), 7.15 – 7.09 (m, 1H), 7.10 – 7.01 (m, 1H), 4.74 (d, $J = 6.2$ Hz, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 162.0, 160.1, 155.6, 155.3, 151.3, 140.5, 130.4, 129.8, 127.4, 125.6, 124.5, 124.0, 121.2, 115.6, 115.5, 111.6, 73.8. $^{19}$F NMR (471 MHz, CDCl$_3$) $\delta$ -60.4. HRMS (ESI, m/z) calcd for C$_{15}$H$_{11}$FN$_2$O$_2$[M+H]$^+$: 271.0877; found: 271.0878.

**N-(3-chlorobenzyl)benzo[d]oxazole-2-carboxamide (5k)**

Compound 5k was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 57% yield (49 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.76 (d, $J = 8.0$ Hz, 1H), 7.70 (s, 1H), 7.65 (d, $J = 8.2$ Hz, 1H), 7.48 (t, $J = 7.8$ Hz, 1H), 7.42 (t, $J = 7.7$ Hz, 1H), 7.36 (s, 1H), 7.29 – 7.26 (m, 2H), 7.25 (d, $J = 4.3$ Hz, 1H), 4.67 (d, $J = 6.2$ Hz, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 155.7, 155.2, 151.2, 140.1, 139.1, 134.7, 130.5, 128.1, 127.5, 126.1, 125.7, 121.2, 111.9, 43.2. HRMS (ESI, m/z) calcd for C$_{15}$H$_{12}$ClN$_2$O$_2$[M+H]$^+$: 287.0582; found: 287.0584.

**N-(3-bromobenzyl)benzo[d]oxazole-2-carboxamide (5l)**

Compound 5l was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 67% yield (67 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.81 (s, 1H), 7.75 – 7.69 (m, 1H), 7.66 – 7.56 (m, 1H), 7.49 (t, $J = 1.6$ Hz, 1H), 7.48 – 7.43 (m, 1H), 7.43 – 7.33 (m, 2H), 7.29 – 7.26 (m, 1H), 7.18 (t, $J = 7.8$ Hz, 1H), 4.65 (d, $J = 6.2$ Hz, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 155.7, 155.2, 151.1, 140.0, 139.4, 131.0, 130.4, 127.5, 126.5, 125.6, 122.8, 121.2, 111.9, 43.2. HRMS (ESI, m/z) calcd for C$_{15}$H$_{11}$BrN$_2$O$_2$[M+H]$^+$: 331.0077; found: 331.0076.
**N-isopropylbenzo[\textit{d}]oxazole-2-carboxamide (5m) (CAS Number: 27383-73-9)**

Compound 5m was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 54% yield (33 mg). 

$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.77 (d, $J = 7.7$ Hz, 1H), 7.65 (d, $J = 8.2$ Hz, 1H), 7.50 – 7.38 (m, 2H), 7.14 (s, 1H), 4.42 – 4.23 (m, 1H), 1.31 (d, $J = 6.6$ Hz, 6H). 

$^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 155.7, 154.8, 151.1, 140.1, 127.3, 125.5, 121.1, 111.9, 42.2, 29.7, 22.6.

**N-butylbenzo[\textit{d}]oxazole-2-carboxamide (5n) (CAS Number: 27383-75-1)**

Compound 5n was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 59% yield (39 mg). 

$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.81 – 7.72 (m, 1H), 7.65 (d, $J = 8.1$ Hz, 1H), 7.50 – 7.39 (m, 2H), 7.31 (s, 1H), 3.55 – 3.46 (m, 2H), 1.68 – 1.60 (m, 2H), 1.48 – 1.39 (m, 2H), 0.96 (t, $J = 7.4$ Hz, 3H).

$^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 155.7, 151.1, 140.2, 127.3, 125.5, 121.1, 111.9, 39.6, 31.4, 29.7, 20.0, 13.7.

**N-isobutylbenzo[\textit{d}]oxazole-2-carboxamide (5o) (CAS Number: 27383-76-2)**

Compound 5o was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow oil in 49% yield (32 mg). 

$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.78 (d, $J = 7.9$ Hz, 1H), 7.69 – 7.62 (m, 1H), 7.49 – 7.40 (m, 2H), 7.37 (s, 1H), 3.38 – 3.31 (m, 2H), 1.99 – 1.89 (m, 1H), 1.02 – 0.97 (m, 6H). 

$^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 155.7 (d, $J = 14.4$ Hz), 151.1, 140.1, 127.3, 125.5, 121.1, 111.9, 47.1, 29.7, 28.6, 20.1.
N-(tert-butyl)benzo[d]oxazole-2-carboxamide (5p) (CAS Number: 95114-65-1)

Compound 5p was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 39% yield (26 mg).

$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.81 – 7.71 (m, 1H), 7.68 – 7.55 (m, 1H), 7.51 – 7.32 (m, 2H), 7.15 (s, 1H), 1.50 (s, 9H).

$^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 156.1, 154.8, 151.2, 140.1, 127.2, 125, 121.0, 111.8, 52.4, 28.6.

N-cyclopropylbenzo[d]oxazole-2-carboxamide (5q) (CAS Number: 1511739-08-4)

Compound 5q was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 67% yield (41 mg).

$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.73 (d, $J$ = 7.7 Hz, 1H), 7.62 (d, $J$ = 8.1 Hz, 1H), 7.48 – 7.34 (m, 3H), 3.02 – 2.88 (m, 1H), 0.93 – 0.88 (m, 2H), 0.73 – 0.69 (m, 2H).

$^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 156.9, 155.4, 151.1, 140.1, 127.4, 125.5, 121.1, 111.9, 22.9, 6.8.

N-((3s,5s,7s)-adamantan-1-yl)benzo[d]oxazole-2-carboxamide (5r)

Compound 5r was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 44% yield (39 mg).

$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.78 – 7.72 (m, 1H), 7.63 (d, $J$ = 7.9 Hz, 1H), 7.46 – 7.38 (m, 2H), 7.02 (s, 1H), 2.15 (s, 9H), 1.76 – 1.68 (m, 6H).

$^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 156.2, 154.4, 151.2, 140.2, 127.1, 125.4, 121.0, 111.8, 53.1, 41.3, 36.2, 29.4. HRMS (ESI, m/z) calcd for C$_{18}$H$_{21}$N$_2$O$_2$[M+H]$^+$: 297.1598; found: 297.1601.
**N-dodecylbenzo[d]oxazole-2-carboxamide (5s) (CAS Number: 50486-32-3)**

Compound 5s was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a white solid in 44% yield (44 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.78 (d, $J = 7.4$ Hz, 1H), 7.65 (d, $J = 8.2$ Hz, 1H), 7.51 – 7.37 (m, 2H), 7.30 (s, 1H), 3.55 – 3.43 (m, 2H), 1.25 (s, 12H), 0.87 (t, $J = 7.0$ Hz, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 155.6 (d, $J = 2.7$ Hz), 151.1, 140.2, 127.3, 125.5, 121.1, 111.9, 39.9, 31.9, 29.7 – 29.2, 26.9, 22.7, 14.1.

**N-allylbenzo[d]oxazole-2-carboxamide (5t) (CAS Number: 27383-71-7)**

Compound 5t was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 45% yield (27 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.81 – 7.75 (m, 1H), 7.65 (d, $J = 8.1$ Hz, 1H), 7.51 – 7.45 (m, 1H), 7.45 – 7.35 (m, 2H), 6.02 – 5.85 (m, 1H), 5.36 – 5.27 (m, 1H), 5.27 – 5.17 (m, 1H), 4.16 – 4.11 (m, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 155.5, 151.2, 140.1, 132.9, 127.4, 125.6, 121.2, 117.5, 111.9, 77.3, 77.0, 76.8, 42.1, 29.7.

**benzo[d]oxazol-2-yl(pyrrrolidin-1-yl)methanone (5u) (CAS Number: 50486-33-4)**

Compound 5u was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 63% yield (41 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.83 – 7.75 (m, 1H), 7.63 (d, $J = 8.1$ Hz, 1H), 7.47 – 7.42 (m, 1H), 7.41 – 7.35 (m, 1H), 4.11 (t, $J = 6.8$ Hz, 2H), 3.73 (t, $J = 6.9$ Hz, 2H), 2.06 – 1.99 (m, 2H), 1.99 – 1.91 (m, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 155.7, 155.3, 150.0, 140.6, 127.1, 125.1, 121.4, 111.6, 49.3, 47.5, 26.5, 23.9.
\textit{N,N-diethylbenzo[d]oxazole-2-carboxamide (5v) (CAS Number: 27383-70-6)}

Compound 5v was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow oil in 38\% yield (25 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.83 – 7.77 (m, 1H), 7.62 (d, $J = 8.0$ Hz, 1H), 7.51 – 7.33 (m, 2H), 3.84 (q, $J = 7.1$ Hz, 2H), 3.61 (q, $J = 7.1$ Hz, 2H), 1.34 – 1.26 (m, 6H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 157.2, 155.4, 149.9, 140.4, 126.9, 125.1, 121.3, 111.5, 43.4, 41.3, 14.6, 12.6.

\textit{N,N-dipropylbenzo[d]oxazole-2-carboxamide (5w) (CAS Number: 27383-74-0)}

Compound 5w was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow oil in 39\% yield (29 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.82 – 7.77 (m, 1H), 7.62 (d, $J = 8.0$ Hz, 1H), 7.47 – 7.38 (m, 2H), 3.77 – 3.72 (m, 2H), 3.53 – 3.48 (m, 2H), 1.74 – 1.70 (m, 4H), 0.98 (t, $J = 7.4$ Hz, 3H), 0.88 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 157.7, 155.5, 149.9, 140.3, 126.8, 125.1, 121.2, 111.4, 50.5, 48.5, 22.4, 20.6, 11.4 11.0.

\textit{6-acetyl-N-isopropylbenzo[d]oxazole-2-carboxamide (5x)}

Compound 5x was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 43\% yield (32 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.11 – 8.01 (m, 1H), 8.00 – 7.85 (m, 1H), 7.51 (t, $J = 7.9$ Hz, 1H), 7.18 (d, $J = 7.0$ Hz, 1H), 4.47 – 4.18 (m, 1H), 2.89 (s, 3H), 1.32 (d, $J = 6.6$ Hz, 6H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 194.4, 156.2, 154.2, 149.6, 141.3, 127.8, 126.1, 125.6, 122.7, 42.4, 30.7, 29.7, 22.5. HRMS (ESI, m/z) calcd for C$_{13}$H$_{15}$N$_2$O$_3$[M+H]$^+$: 247.1077; found: 247.1079.
6-methyl-N-phenylbenzo[d]oxazole-2-carboxamide (5y) (CAS Number: 1539536-18-9)

Compound 5y was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a white solid in 68% yield (51 mg). $^1$H NMR (500 MHz, CDCl$_3$) δ 9.08 (s, 1H), 7.75 – 7.72 (m, 2H), 7.45 (s, 1H), 7.42 – 7.37 (m, 2H), 7.25 (d, $J$ = 9.8 Hz, 1H), 7.19 (t, $J$ = 7.4 Hz, 1H), 2.51 (s, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 155.1, 153.4, 151.8, 138.6, 137.9, 136.9, 129.3, 127.3, 125.2, 120.5, 119.9, 111.9, 22.0.

5-methoxy-N-phenylbenzo[d]oxazole-2-carboxamide (5z) (CAS Number: 1504693-37-1)

Compound 5za was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 34% yield (27 mg). $^1$H NMR (500 MHz, CDCl$_3$) δ 9.07 (s, 1H), 7.74 (d, $J$ = 7.7 Hz, 2H), 7.55 (d, $J$ = 9.0 Hz, 1H), 7.40 (t, $J$ = 8.0 Hz, 2H), 7.23 (d, $J$ = 2.5 Hz, 1H), 7.20 (t, $J$ = 7.4 Hz, 1H), 7.14 – 7.05 (m, 1H), 3.87 (s, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 158.2, 156.1, 153.2, 146.2, 140.9, 136.8, 129.3, 125.3, 119.9, 117.2, 112.2, 103.0, 56.0.

ethyl benzo[d]oxazole-2-carboxylate (5za) (CAS Number: 27383-87-5)

Compound 5zd was prepared according to the general procedure (petroleum ether/ethyl acetate = 10:1 v/v). The product was obtained as a yellow solid in 42% yield (24 mg). $^1$H NMR (500 MHz, CDCl$_3$) δ 7.89 (d, $J$ = 8.0 Hz, 1H), 7.66 (d, $J$ = 8.3 Hz, 1H), 7.55 – 7.50 (m, 1H), 7.48 – 7.40 (m, 1H), 4.56 (q, $J$ = 7.1 Hz, 2H), 1.49 (t, $J$ = 7.1 Hz, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 156.5, 152.8, 150.9, 140.5, 128.2, 125.8, 122.2, 111.8, 63.3, 14.2.

N-phenylbenzo[d]thiazole-2-carboxamide (7a) (CAS Number: 68070-62-2)
Compound 7a was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 85% yield (43 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 9.29 (s, 1H), 8.11 (d, $J$ = 8.2 Hz, 1H), 7.97 (d, $J$ = 8.0 Hz, 1H), 7.77 (d, $J$ = 7.7 Hz, 2H), 7.60 – 7.48 (m, 2H), 7.40 (t, $J$ = 7.9 Hz, 2H), 7.19 (t, $J$ = 7.4 Hz, 1H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 164.1, 157.6, 152.7, 137.4, 129.3, 127.0, 125.0, 124.4, 122.5, 119.8.

N-(4-fluorophenyl)benzo[d]thiazole-2-carboxamide (7b) (CAS Number: 801242-43-3)

Compound 7b was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a white solid in 80% yield (44 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 9.27 (s, 1H), 8.10 (d, $J$ = 8.2 Hz, 1H), 7.98 (d, $J$ = 8.0 Hz, 1H), 7.78 – 7.67 (m, 2H), 7.59 – 7.56 (m, 1H), 7.54 – 7.48 (m, 1H), 7.11 – 7.07 (m, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 163.8, 160.7, 158.8, 157.6, 152.6, 137.4, 133.1, 127.1, 124.4, 122.6 – 122.3, 121.6, 116.2, 116.0, 115.9. $^{19}$F NMR (471 MHz, CDCl$_3$) $\delta$ -116.89 (s).

N-(4-chlorophenyl)benzo[d]thiazole-2-carboxamide (7c) (CAS Number: 801242-43-3)

Compound 7c was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 65% yield (37 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 9.27 (s, 1H), 8.08 (d, $J$ = 8.1 Hz, 1H), 7.96 (d, $J$ = 7.9 Hz, 1H), 7.73 – 7.67 (m, 2H), 7.59 – 7.47 (m, 2H), 7.37 – 7.31 (m, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 163.6, 157.6, 152.6, 137.4, 135.6, 130.0, 129.3, 127.1, 124.4, 122.5, 121.0.

N-(p-tolyl)benzo[d]thiazole-2-carboxamide (7d) (CAS Number: 68070-63-3)
Compound 7d was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a white solid in 55% yield (30 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 9.22 (s, 1H), 8.13 – 8.09 (m, 1H), 7.98 (d, $J$ = 8.0 Hz, 1H), 7.67 – 7.63 (m, 2H), 7.59 – 7.55 (m, 1H), 7.53 – 7.49 (m, 1H), 7.20 (d, $J$ = 8.2 Hz, 2H), 2.35 (s, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 164.3, 157.5, 152.7, 137.4, 134.7, 134.5, 129.8, 126.9, 124.3, 122.5, 120.5, 119.8, 21.0.

N-(4-methoxyphenyl)benzo[d]thiazole-2-carboxamide (7e) (CAS Number: 722461-39-4)

Compound 7e was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 83% yield (47 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 9.19 (s, 1H), 8.10 (d, $J$ = 8.2 Hz, 1H), 7.98 (d, $J$ = 8.0 Hz, 1H), 7.73 – 7.64 (m, 2H), 7.60 – 7.46 (m, 2H), 6.93 (d, $J$ = 9.0 Hz, 2H), 3.82 (s, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 164.3, 157.3, 156.8, 152.7, 137.4, 134.7, 130.2, 126.9, 124.3, 122.5, 121.4, 114.4, 55.5.

N-(2-methylbenzyl)benzo[d]thiazole-2-carboxamide (7f)

Compound 7f was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 90% yield (51 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.06 – 7.99 (m, 1H), 8.00 – 7.94 (m, 1H), 7.62 (s, 1H), 7.57 – 7.45 (m, 2H), 7.38 – 7.30 (m, 1H), 7.26 – 7.17 (m, 3H), 4.70 (d, $J$ = 5.8 Hz, 2H), 2.40 (s, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 163.7, 159.7, 152.9, 137.1, 136.6, 135.0, 130.7, 128.9, 128.1, 126.8, 126.4, 124.3, 122.4, 42.1, 19. HRMS (ESI, m/z) calcd for C$_{16}$H$_{15}$N$_2$OS[M+H]$^+$: 283.0900; found: 283.0897.

N-(3-chlorobenzyl)benzo[d]thiazole-2-carboxamide (7g)
Compound 7g was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a colorless oil in 57% yield (34 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 8.06 – 8.00 (m, 1H), 8.00 – 7.94 (m, 1H), 7.87 (s, 1H), 7.56 – 7.47 (m, 2H), 7.36 (s, 1H), 7.28 – 7.25 (m, 3H), 4.66 (d, \(J = 6.2\) Hz, 2H). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 163.4, 160.0, 152.8, 139.5, 137.1, 134.7, 130.1, 128.0 (t, \(J = 3.6\) Hz), 126.9 (d, \(J = 6.4\) Hz), 126.1, 124.3, 122.4, 43.3. HRMS (ESI, m/z) calcd for C\(_{15}\)H\(_{11}\)ClN\(_2\)OS[M+H]\(^+\): 303.0353; found: 303.0354.

N-(3-methylbenzyl)benzo[d]thiazole-2-carboxamide (7h)

Compound 7h was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 84% yield (47 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 8.06 – 8.00 (m, 1H), 8.00 – 7.95 (m, 1H), 7.78 (s, 1H), 7.59 – 7.43 (m, 2H), 7.25 (2, \(J = 7.4\), 4.6 Hz, 1H), 7.22 – 7.14 (m, 2H), 7.15 – 7.08 (m, 1H), 4.66 (d, \(J = 6.0\) Hz, 2H), 2.35 (d, \(J = 5.7\) Hz, 3H). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 163.8, 159.8, 152.9, 138.6, 137.2, 128.8, 126.8, 125.1, 124.3, 122.4, 43.9, 21.4. HRMS (ESI, m/z) calcd for C\(_{16}\)H\(_{15}\)N\(_2\)OS[M+H]\(^+\): 283.0900; found: 283.0904.

N-benzylbenzo[d]thiazole-2-carboxamide (7i) (CAS Number: 148149-23-9)

Compound 7i was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 55% yield (30 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 8.03 (d, \(J = 8.2\) Hz, 1H), 7.97 (d, \(J = 7.9\) Hz, 1H), 7.79 (s, 1H), 7.57 – 7.46 (m, 2H), 7.42 – 7.34 (m, 4H), 7.32 (d, \(J = 6.9\) Hz, 1H), 4.70 (d, \(J = 6.1\) Hz, 2H). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 163.6, 159.8, 152.9, 137.4, 137.1, 128.9, 128.1 – 127.6, 126.8, 124.8, 122.4, 43.9.

N-isopropylbenzo[d]thiazole-2-carboxamide (7j) (CAS Number: 41124-28-1)
Compound 7j was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 54% yield (24 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.09 – 8.00 (m, 1H), 7.99 – 7.85 (m, 1H), 7.56 – 7.51 (m, 1H), 7.51 – 7.45 (m, 1H), 7.28 (d, $J$ = 5.2 Hz, 1H), 4.36 – 4.23 (m, 1H), 1.32 (d, $J$ = 6.6 Hz, 6H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 164.5, 159.0, 152.9, 137.1, 126.7, 124.1 122.4, 42.2, 22.7.

N-butylbenzo[d]thiazole-2-carboxamide (7k) (CAS Number: 41039-01-4)

Compound 7k was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 78 % yield (37 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.05 (d, $J$ = 8.2 Hz, 1H), 7.96 (d, $J$ = 8.0 Hz, 1H), 7.57 – 7.51 (m, 1H), 7.51 – 7.39 (m, 2H), 3.55 – 3.47 (m, 2H), 1.69 – 1.62 (m, 2H), 1.49 – 1.40 (m, 2H), 0.97 (t, $J$ = 7.4 Hz, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 164.3, 159.9, 152.9, 137.1, 126.7, 124.2, 122.4, 39.6, 31.6, 20.1, 13.7.

N-(tert-butyl)benzo[d]thiazole-2-carboxamide (7l) (CAS Number: 41039-02-5)

Compound 7l was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow oil in 77 % yield (36 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.04 (d, $J$ = 8.2 Hz, 1H), 7.96 (d, $J$ = 8.0 Hz, 1H), 7.61 – 7.50 (m, 1H), 7.49 – 7.41 (m, 1H), 7.33 (s, 1H), 1.52 (s, 9H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 165.6, 159.0, 152.9, 137.2, 126.7, 126.5, 124.1, 122.4, 52.1, 28.7.

5-chloro-N-dodecylbenzo[d]thiazole-2-carboxamide (7m)
Compound 7m was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 76% yield (25 mg). 
$^1$H NMR (500 MHz, CDCl$_3$) δ 8.05 (d, $J = 8.2$ Hz, 1H), 7.95 (d, $J = 8.0$ Hz, 1H), 7.56 – 7.50 (m, 1H), 7.51 – 7.44 (m, 2H), 3.52 – 3.46 (m, 2H), 1.24 (s, 18H), 0.89 – 0.84 (m, 5H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 164.2, 159.8, 152.9, 137.1, 126.7, 124.2, 122.4, 40.3, 39.9, 31.9, 29.7 – 29.1, 29.0, 26.9, 26.7, 22.7, 14.1. HRMS (ESI, m/z) calcd for C$_{20}$H$_{29}$ClN$_2$OS$^{[M+H]^+}$: 381.1762; found: 381.1761.

N,N-diethylbenzo[d]thiazole-2-carboxamide (7n) (CAS Number: 673485-50-2)

Compound 7n was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow oil in 41% yield (19 mg). $^1$H NMR (500 MHz, CDCl$_3$) δ 8.14 – 8.03 (m, 1H), 7.99 – 7.85 (m, 1H), 7.62 – 7.36 (m, 2H), 4.07 (q, $J = 7.0$ Hz, 2H), 3.60 (q, $J = 7.1$ Hz, 2H), 1.34 – 1.27 (m, 6H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 165.2, 160.6, 153.4, 136.2, 126.4, 124.6, 121.8, 43.2, 42.3, 14.6, 12.7.

N,N-dipropylbenzo[d]thiazole-2-carboxamide (7o) (CAS Number: 1024441-13-1)

Compound 7o was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow oil in 38% yield (20 mg). $^1$H NMR (500 MHz, CDCl$_3$) δ 8.07 (d, $J = 8.2$ Hz, 1H), 7.95 (d, $J = 7.9$ Hz, 1H), 7.60 – 7.41 (m, 2H), 4.08 – 3.91 (m, 2H), 3.58 – 3.42 (m, 2H), 1.82 – 1.68 (m, 4H), 0.98 (t, $J = 7.4$ Hz, 3H), 0.92 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 165.4, 161.0, 153.4, 136.3, 126.4, 124.6, 121.8, 50.3, 49.8, 22.6, 20.8, 11.5, 11.0.
N,N-dibenzylbenzo[d]thiazole-2-carboxamide (7p)

Compound 7p was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a white solid in 32 % yield (23 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.06 – 8.00 (m, 1H), 8.00 – 7.95 (m, 1H), 7.53 – 7.46 (m, 2H), 7.41 – 7.28 (m, 10H), 5.42 (s, 2H), 4.72 (s, 2H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 164.8, 161.5, 153.2, 136.8, 136.4 (d, $\text{J}$ = 15.4 Hz), 128.7 (d, $\text{J}$ = 18.0 Hz), 127.9, 127.7, 126.8, 126.5, 124.8, 121.8 50.5, 49.1. HRMS (ESI, m/z) calcd for C$_{22}$H$_{19}$N$_2$OS[$\text{M+H}^+$]: 359.1213; found: 359.1212.

benzo[d]thiazol-2-yl(morpholino)methanone (7q) (CAS Number: 78224-61-0)

Compound 7m was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 72 % yield (36 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.07 (d, $\text{J}$ = 8.1 Hz, 1H), 7.95 (d, $\text{J}$ = 7.8 Hz, 1H), 7.56 – 7.46 (m, 2H), 4.56 – 4.47 (m, 2H), 3.87 – 3.79 (m, 6H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 164.5, 159.7, 153.1, 136.2, 126.8, 126.6, 124.6, 121.87 (s), 67.2, 66.9, 47.2, 43.9.

5-chloro-N,N-diethylbenzo[d]thiazole-2-carboxamide (7r)

Compound 7r was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a white solid in 47% yield (25 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.13 – 8.05 (m, 1H), 7.90 – 7.82 (m, 1H), 7.49 – 7.41 (m, 1H), 4.05 (q, $\text{J}$ = 7.0 Hz, 2H), 3.59 (q, $\text{J}$ = 7.1 Hz, 2H), 1.34 – 1.27 (m, 6H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 167.2, 160.1, 154.2, 134.6, 132.4, 127.1, 124.3, 122.6, 43.2, 42.5, 14.6, 12.7. HRMS (ESI, m/z) calcd for C$_{16}$H$_{15}$N$_2$OS[$\text{M+H}^+$]: 269.0510; found: 269.0513.

5-chloro-N,N-dipropylbenzo[d]thiazole-2-carboxamide (7s)
 Compound 7s was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 65% yield (39 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 8.08 – 8.03 (m, 1H), 7.85 (d, \(J = 8.6\) Hz, 1H), 7.46 – 7.41 (m, 1H), 4.02 – 3.92 (m, 2H), 3.53 – 3.43 (m, 2H), 1.78 – 1.69 (m, 4H), 1.00 – 0.90 (m, 6H). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 167.5, 160.4, 154.2, 134.6, 132.4, 127.1, 124.3, 122.6, 50.3, 49.9, 22.6, 20.8, 11.5, 11.0. HRMS (ESI, m/z) calcd for \(\text{C}_{14}\text{H}_{17}\text{ClN}_2\text{OS}[\text{M+H}]^+\): 297.0823; found: 297.0821.

**ethyl benzo[d]thiazole-2-carboxylate (7t) (CAS Number: 32137-76-1)**

 Compound 7t was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 75% yield (31 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 8.38 – 8.15 (m, 1H), 8.09 – 7.81 (m, 1H), 7.61 – 7.47 (m, 2H), 4.54 (q, \(J = 7.1\) Hz, 2H), 1.48 (t, \(J = 7.1\) Hz, 3H). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 160.7, 158.6, 153.2, 136.8, 127.5, 127.1, 125.5, 122.1, 63.1, 14.3.

**ethyl 5-chlorobenzo[d]thiazole-2-carboxylate (7u) (CAS Number: 857081-41-5)**

 Compound 7u was prepared according to the general procedure (petroleum ether/ethyl acetate = 20:1 v/v). The product was obtained as a yellow solid in 46% yield (22 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 8.20 (d, \(J = 1.8\) Hz, 1H), 7.88 (d, \(J = 8.6\) Hz, 1H), 7.56 – 7.42 (m, 1H), 4.54 (q, \(J = 7.1\) Hz, 2H), 1.48 (t, \(J = 7.1\) Hz, 3H). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 160.3 (d, \(J = 8.5\) Hz), 153.9, 135.0, 133.3, 128.2, 125.0, 122.9, 63.3, 14.3.

**8. References**

9. NMR spectroscopic data
N-isopropyl-1H-benzo[d]imidazole-2-carboxamide (3a)

N-(tert-butyl)-1H-benzo[d]imidazole-2-carboxamide (3b)
N-benzyl-1H-benzo[d]imidazole-2-carboxamide (3c)
O-allyl-1H-benzo[d]imidazole-2-carboxamide (3d)
N-phenyl-1H-benzo[d]imidazole-2-carboxamide (3e)
N-cyclopropyl-1H-benzo[d]imidazole-2-carboxamide (3f)

(1H-benzo[d]imidazol-2-yl)(pyrrolidin-1-yl)methanone (3g)
N,N-diethyl-1H-benzo[d]imidazole-2-carboxamide (3h)
N,N-dibenzyl-1H-benzo[d]imidazole-2-carboxamide (3i)
N-isopropyl-5-methyl-1H-benzo[d]imidazole-2-carboxamide (3j)
O-isopropyl-5,6-dimethyl-1H-benzo[d]imidazole-2-carboxamide (3k)
5-chloro-N-isopropyl-1H-benzo[d]imidazole-2-carboxamide (3l)
N-isopropyl-5-nitro-1H-benzo[d]imidazole-2-carboxamide (3m)
N-isopropyl-5-(trifluoromethyl)-1H-benzo[d]imidazole-2-carboxamide (3n)
ethyl 1H-benzo[d]imidazole-2-carboxylate (3o)
N-phenylbenzo[d]oxazole-2-carboxamide (5a)
N-(4-methoxyphenyl)benzo[d]oxazole-2-carboxamide (5b)
N-(p-tolyl)benzo[d]oxazole-2-carboxamide (5c)
N-(4-fluorophenyl)benzo[d]oxazole-2-carboxamide (5d)
N-(4-chlorophenyl)benzoxazole-2-carboxamide (5e)
$N$-(2-methylbenzyl)benzo[\textit{d}]oxazole-2-carboxamide (5f)
$N$-(3-methylbenzyl)benzo[d]oxazole-2-carboxamide (5g)
N-(4-methoxybenzyl)benzo[d]oxazole-2-carboxamide (5h)
N-benzylbenzoxazole-2-carboxamide (5i)
$N$-(2-fluorobenzyl)benzo[d]oxazole-2-carboxamide (5j)
\textit{N-(3-chlorobenzyl)benzo[d]oxazole-2-carboxamide} (5k)
N-(3-bromobenzyl)benzo[d]oxazole-2-carboxamide (5l)
$N$-isopropylbenzo[d]oxazole-2-carboxamide (5m)
$N$-butylbenzo[d]oxazole-2-carboxamide (5n)
N-isobutylbenzo[\textit{d}]oxazole-2-carboxamide (5o)
N-(tert-butyl)benzo[d]oxazole-2-carboxamide (5p)
N-cyclopropylbenzo[d]oxazole-2-carboxamide (5q)
N-((3s,5s,7s)-adamantan-1-yl)benzo[d]oxazole-2-carboxamide (5r)
N-dodecylbenzo[d]oxazole-2-carboxamide (5s)
$N$-allylbenzo[\textit{d}]oxazole-2-carboxamide (5t)
benzo[d]oxazol-2-yl(pyrrolidin-1-yl)methanone (5u)
$N,N$-diethylbenzo[$d$]oxazole-2-carboxamide (5v)
N,N-dipropylbenzodioxazole-2-carboxamide (5w)
6-acetyl-N-isopropylbenzo[\textit{d}]oxazole-2-carboxamide (5x)
6-methyl-N-phenylbenzo\[d\]oxazole-2-carboxamide (5y)
5-methoxy-N-phenylbenzo[d]oxazole-2-carboxamide (5z)
ethyl benzo[d]oxazole-2-carboxylate (5za)
N-phenylbenzo[d]thiazole-2-carboxamide (7a)
N-(4-fluorophenyl)benzo[d]thiazole-2-carboxamide (7b)
N-(4-chlorophenyl)benzo[d]thiazole-2-carboxamide (7c)
N-(p-tolyl)benzo[d]thiazole-2-carboxamide (7d)
N-(4-methoxyphenyl)benzo[d]thiazole-2-carboxamide(7e)
N-(2-methylbenzyl)benzo[d]thiazole-2-carboxamide (7f)
N-(3-chlorobenzyl)benzo[d]thiazole-2-carboxamide (7g)
N-(3-methylbenzyl)benzo[d]thiazole-2-carboxamide (7h)
N-benzylbenzo[d]thiazole-2-carboxamide (7i)
N-isopropylbenzo[d]thiazole-2-carboxamide (7j)
N-butylbenzo[d]thiazole-2-carboxamide (7k)
N-(tert-butyl)benzo[d]thiazole-2-carboxamide (7l)
5-chloro-N-dodecylbenzo[d]thiazole-2-carboxamide (7m)
N,N-diethylbenzo[d]thiazole-2-carboxamide (7n)
N,N-dipropylbenzo[d]thiazole-2-carboxamide (7o)
N,N-dibenzylbenzo[d]thiazole-2-carboxamide (7p)
benzo[d]thiazol-2-yl(morpholino)methanone (7q)
5-chloro-N,N-diethylbenzo[d]thiazole-2-carboxamide (7r)
5-chloro-N,N-dipropylbenzo[d]thiazole-2-carboxamide (7s)
ethyl benzo[d]thiazole-2-carboxylate (7t)
ethyl 5-chlorobenzo[d]thiazole-2-carboxylate (7u)