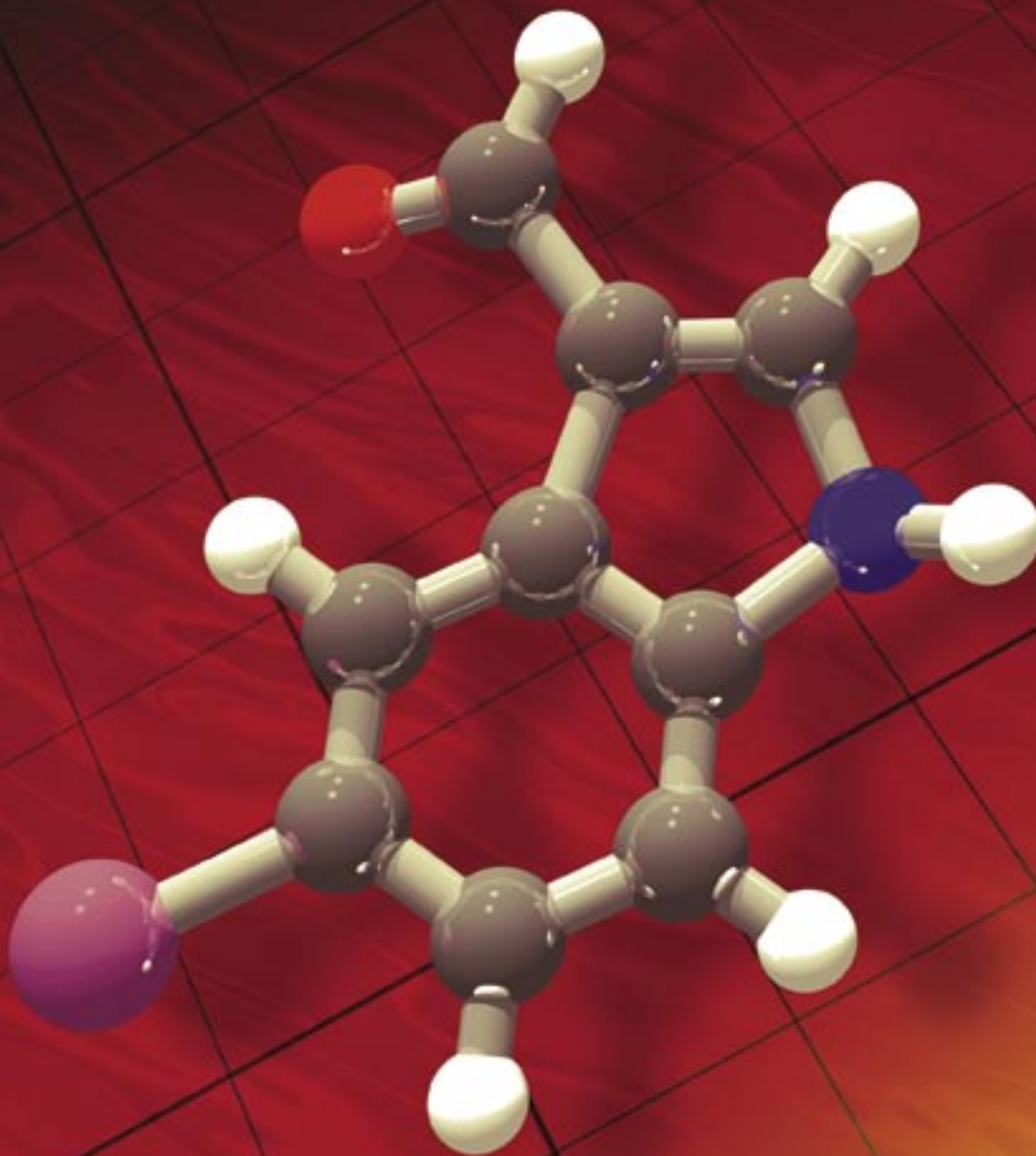


Privileged Structures for Lead
Discovery and Optimization

Indoles

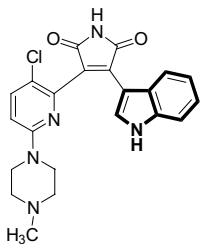


Privileged Structures: Indoles

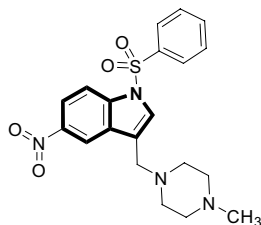
Sigma-Aldrich is proud to offer a new series of *ChemFiles*—called Privileged Structures, to our Drug Discovery and Organic Synthesis customers. Each piece will highlight a specific motif, selected applications, and the range of products Sigma-Aldrich offers in this area. Our first installment focuses on the indole scaffold. In the future we will be highlighting other medicinally relevant cores and other selected drug-relevant building blocks. We trust you will find these pieces useful, and we welcome your comments for future installments. If you do not see a particular product or wish to have us synthesize one for you, please email us at DrugDiscovery@sial.com.

Privileged structures are described as a class of molecules capable of binding to multiple receptors with high affinity.¹ Utilization of these molecules enables the medicinal chemist to rapidly determine biologically active compounds across a wide range of therapeutic areas. In practice, the medicinal chemist will often choose to synthesize one library based upon one core scaffold and screen it against a variety of receptors, yielding several active compounds. In order to be considered privileged, a substructure should represent a molecule's core element and make up a significant portion of its total mass.

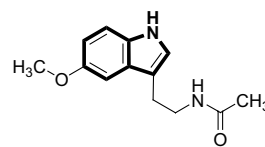
The privileged structure highlighted in this *ChemFile* is the indole scaffold. The indole substructure is a basic element for a number of biologically active natural and synthetic products. Since January 2003, there have been more than 400 drugs and 3000 patents in which the indole motif has been present. The range of applications for these therapeutically relevant compounds includes protein kinase C inhibitors, 5-HT agonists, melatonin agonists, and glucocorticoid receptor modulators.



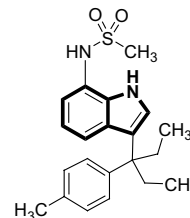
Protein kinase C inhibitor shown to be useful treatment for cardiovascular diseases, diabetes, respiratory disorders, and autoimmune disease²



5-HT agonist useful for treatment of neurological and cognitive disorders³

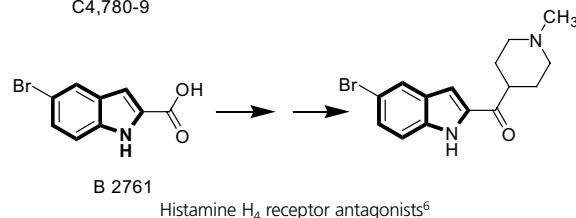
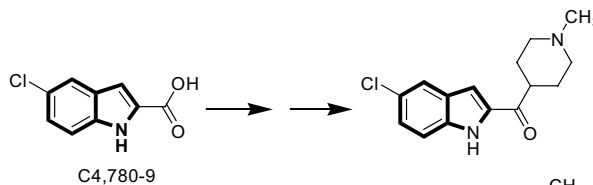


Melatonin agonist useful treatment for strokes⁴

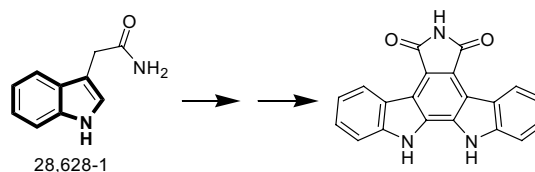


Glucocorticoid receptor modulator useful for treatment of hypertension, arrhythmias, and myocardial infarction⁵

Recent literature illustrates the use of Sigma-Aldrich as starting materials for a number of biologically active compounds. Three examples are listed below.



Histamine H₄ receptor antagonists⁶



Potent Cyclin D1-CDK4 Inhibitor⁷

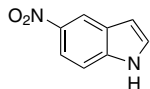
Listed on the following pages is a selection of indoles available from Sigma-Aldrich. For a complete list of indoles, please visit our Web site at sigmaaldrich.com under the Drug Discovery Product lines.

References:

1. *Chem. Rev.* **2003**, *103*, 893–930
2. Novartis AG., Patent number WO-2004072062
3. Suen Life Sciences Limited, WO-2004048330
4. The University of Hong Kong, Ultra Biotech Ltd., WO-2004066995
5. Eli Lilly and Company, WO-2004067529
6. *Bioorganic & Medicinal Chemistry Letter* **2004**, *14*, 5251–5256
7. *J. Med. Chem.* **2003**, *46*, 2027–2030

5-Nitroindole, 98%

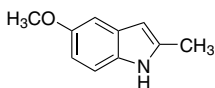
N1,760-2
 $C_8H_6N_2O_2$
 Mw 162.15



1 g
 5 g
 25 g

5-Methoxy-2-methylindole, 99%

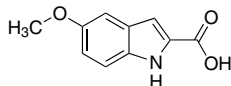
M1,545-1
 $C_{10}H_{11}NO$
 Mw 161.2



1 g
 5 g

5-Methoxyindole-2-carboxylic acid, 97%

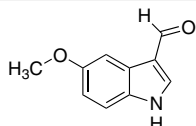
M1,495-1
 $C_{10}H_9NO_3$
 Mw 191.18



1 g
 5 g
 10 g

5-Methoxyindole-3-carboxaldehyde, ≥99%

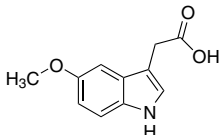
M1,494-3
 $C_{10}H_9NO_2$
 Mw 175.18



100 mg
 1 g

5-Methoxy-3-indoleacetic acid, 98%

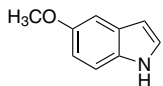
M1,493-5
 $C_{11}H_{11}NO_3$
 Mw 205.21



250 mg
 1 g

5-Methoxyindole, 99%

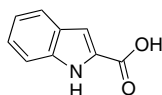
M1,490-0
 C_9H_9NO
 Mw 147.17



1 g
 5 g

Indole-2-carboxylic acid, 98%

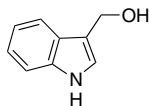
I5109
 $C_9H_7NO_2$
 Mw 161.16



5 g
 10 g
 50 g

Indole-3-carbinol

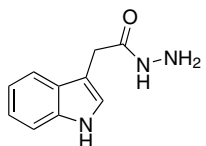
I7256
 C_9H_9NO
 Mw 147.17



1 g
 5 g
 25 g

Indole-3-acetic hydrazide, 97%

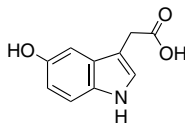
I3777
 $C_{10}H_{11}N_3O$
 Mw 189.21



1 g
 10 g

5-Hydroxyindole-3-acetic acid, ≥98%

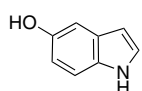
H8876
 $C_{10}H_9NO_3$
 Mw 191.18



100 mg
 500 mg
 1 g \$75.80

5-Indolol, 97%

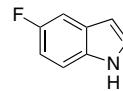
H3,185-9
 C_8H_7NO
 Mw 133.15



250 mg
 1 g

5-Fluoroindole, 98%

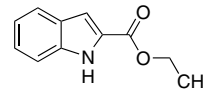
F9108
 C_8H_6FN
 Mw 135.14



250 mg
 1 g

Ethyl indole-2-carboxylate, 97%

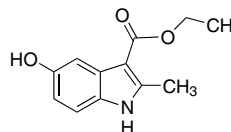
E3,280-0
 $C_{11}H_{11}NO_2$
 Mw 189.21



5 g
 25 g

Ethyl 5-hydroxy-2-methylindole-3-carboxylate, 97%

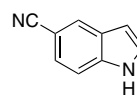
E3,180-4
 $C_{12}H_{13}NO_3$
 Mw 219.24



1 g

Indole-5-carbonitrile, 99%

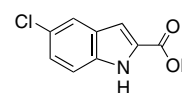
C9,200-6
 $C_9H_6N_2$
 Mw 142.16



250 mg
 1 g
 5 g
 10 g

5-Chloroindole-2-carboxylic acid, 98%

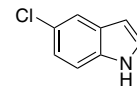
C4,780-9
 $C_9H_6ClNO_2$
 Mw 195.6



1 g
 5 g

5-Chloroindole, 98%

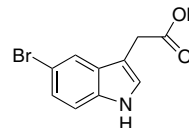
C4,760-4
 C_8H_6ClN
 Mw 151.59



1 g
 5 g

5-Bromoindole-3-acetic acid, 97%

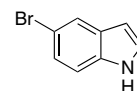
B6,872-0
 $C_{10}H_8BrNO_2$
 Mw 254.08



250 mg
 1 g

5-Bromoindole, 99%

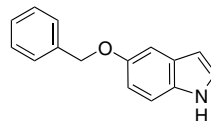
B6,860-7
 C_8H_6BrN
 Mw 196.04



5 g
 25 g

5-Benzyloxyindole, various solvents of crystallization 5%, 95%

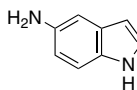
B2,780-3
 $C_{15}H_{13}NO$
 Mw 223.27



1 g
 5 g
 25 g

5-Aminoindole, 97%

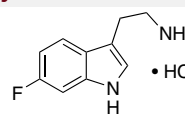
A5,965-4
 $C_8H_8N_2$
 Mw 132.16



250 mg
 1 g
 5 g

6-Fluorotryptamine hydrochloride, 99%

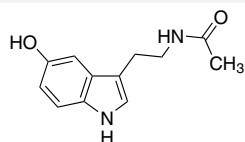
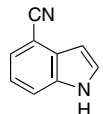
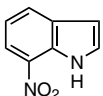
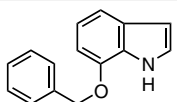
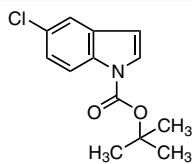
86,025-5
 $C_{10}H_{11}FN_2 \cdot HCl$
 Mw 214.67



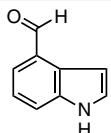
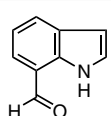
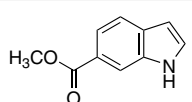
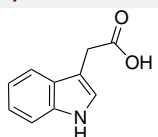
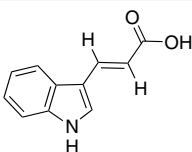
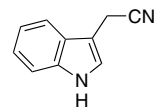
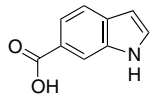
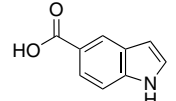
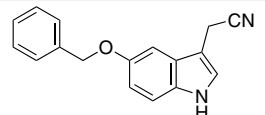
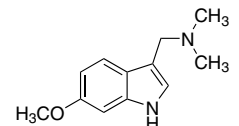
100 mg
 500 mg



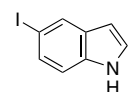
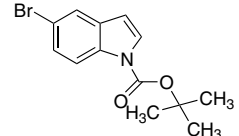
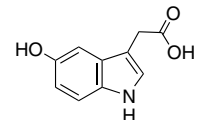
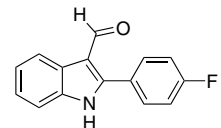
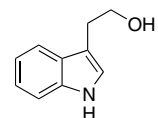
Ready to scale up? For competitive quotes on larger quantities or custom synthesis, contact SAFC at 1-800-244-1173 (USA), or visit safcglobal.com

N-Acetyl-5-hydroxytryptamine, 99%**85,548-0**C₁₂H₁₄N₂O₂
Mw 218.2525 mg
100 mg
250 mg**4-Cyanoindole, 97%****64,553-2**C₉H₆N₂
Mw 142.161 g
5 g**7-Nitroindole, 97%****63,885-4**C₈H₆N₂O₂
Mw 162.151 g
5 g**7-Benzyloxyindole****63,680-0**C₁₅H₁₃NO
Mw 223.271 g
5 g**1-(tert-Butoxycarbonyl)-5-chloroindole, 97%****63,675-4**C₁₃H₁₄ClNO₂
Mw 251.71

1 g

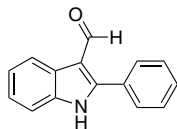
Indole-4-carboxaldehyde, 97%**63,242-2**C₉H₇NO
Mw 145.161 g
5 g**Indole-7-carboxaldehyde, 97%****63,241-4**C₉H₇NO
Mw 145.161 g
5 g**Methyl indole-6-carboxylate, 97%****57,849-5**C₁₀H₉NO₂
Mw 175.181 g
5 g**3-Indoleacetic acid, techn., ≥95% T****57333**C₁₀H₉NO₂
Mw 175.185 g
25 g
100 g**3-Indoleacrylic acid, purum, ≥97.0% HPLC****57290**C₁₁H₉NO₂
Mw 187.191 g
5 g**3-Indoleacetonitrile, purum, ≥96.0% GC****57280**C₁₀H₈N₂
Mw 156.185 g
25 g**Indole-6-carboxylic acid, purum, ≥97.0% T****57235**C₉H₇NO₂
Mw 161.161 g
5 g**Indole-5-carboxylic acid, purum, ≥98.0% T****57230**C₉H₇NO₂
Mw 161.161 g
5 g**(5-Benzyloxyindol-3-yl)acetonitrile, 97%****56,770-1**C₁₇H₁₄N₂O
Mw 262.311 g
5 g**(6-Methoxyindol-3-ylmethyl)dimethylamine, 97%****56,764-7**C₁₂H₁₆N₂O
Mw 204.27

1 g

5-Iodoindole, 98%**56,383-8**C₈H₆IN
Mw 243.045 g
25 g**tert-Butyl 5-bromoindole-1-carboxylate, 97%****55,774-9**C₁₃H₁₄BrNO₂
Mw 296.165 g
25 g**5-Hydroxyindole-3-acetic acid, BioChemika, ≥99.0% HPLC****55360**C₁₀H₉NO₃
Mw 191.18250 mg
1 g**2-(4-Fluorophenyl)-1H-indole-3-carboxaldehyde****54,981-9**C₁₅H₁₀FNO
Mw 239.241 g
5 g**3-(2-Hydroxyethyl)indole purum, ≥98.0% GC****54350**C₁₀H₁₁NO
Mw 161.21 g
5 g

2-Phenylindole-3-carboxaldehyde, 97%

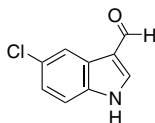
54,332-2
 $C_{15}H_{11}NO$
 Mw 221.25



1 g
 5 g

5-Chloroindole-3-carboxaldehyde, 98%

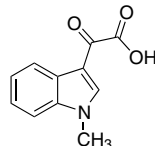
53,307-6
 C_9H_6ClNO
 Mw 179.6



5 g

N-Methyl-3-indoleglyoxylic acid, 97%

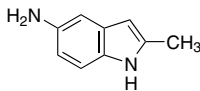
52,587-1
 $C_{11}H_9NO_3$
 Mw 203.19



5 g

5-Amino-2-methylindole, 97%

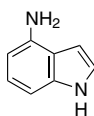
52,558-8
 $C_9H_{10}N_2$
 Mw 146.19



5 g

4-Aminoindole, 97%

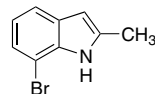
52,502-2
 $C_8H_8N_2$
 Mw 132.16



500 mg

7-Bromo-2-methylindole, 96%

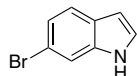
52,486-7
 C_9H_8BrN
 Mw 210.07



1 g
 5 g

6-Bromoindole, 96%

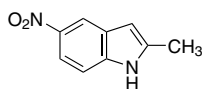
52,434-4
 C_8H_6BrN
 Mw 196.04



250 mg
 1 g

2-Methyl-5-nitroindole, 97%

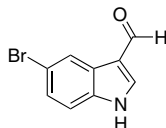
52,059-4
 $C_9H_8N_2O_2$
 Mw 176.17



1 g
 5 g

5-Bromoindole-3-carboxaldehyde, 98%

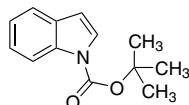
51,874-3
 C_9H_6BrNO
 Mw 224.05



5 g

tert-Butyl 1-indolecarboxylate

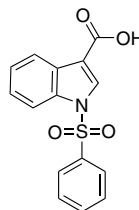
51,810-7
 $C_{13}H_{15}NO_2$
 Mw 217.26



25 mL

1-(Phenylsulfonyl)-3-indolecarboxaldehyde, 97%

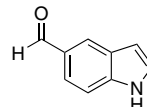
51,641-4
 $C_{15}H_{11}NO_3S$
 Mw 285.32



500 mg
 1 g

Indole-5-carboxaldehyde, 98%

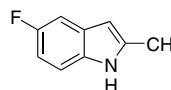
51,383-0
 C_9H_7NO
 Mw 145.16



5 g

5-Fluoro-2-methylindole, 98%

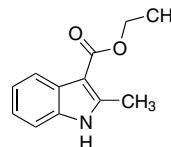
51,153-6
 C_9H_8FN
 Mw 149.16



5 g

Ethyl 2-methylindole-3-carboxylate, 99%

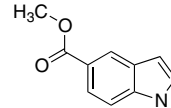
51,141-2
 $C_{12}H_{13}NO_2$
 Mw 203.24



250 mg
 1 g

Methyl indole-5-carboxylate, 99%

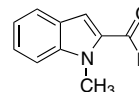
51,118-8
 $C_{10}H_9NO_2$
 Mw 175.18



1 g

1-Methylindole-2-carboxaldehyde, 97%

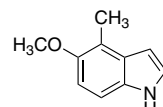
51,112-9
 $C_{10}H_9NO$
 Mw 159.18



5 g

5-Methoxy-4-methylindole, 98%

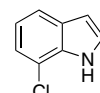
49,723-1
 $C_{10}H_{11}NO$
 Mw 161.2



250 mg
 1 g

7-Chloroindole, 97%

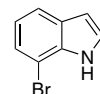
47,373-1
 C_8H_6ClN
 Mw 151.59



1 g

7-Bromoindole, 96%

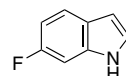
47,372-3
 C_8H_6BrN
 Mw 196.04



250 mg
 1 g
 5 g

6-Fluoroindole, purum, ≥98.0% GC

47085
 C_8H_6FN
 Mw 135.14



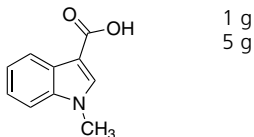
250 mg
 1 g



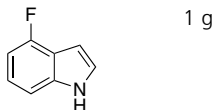
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1-Methylindole-3-carboxylic acid, 97%

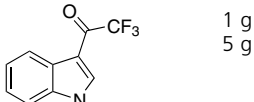
46,531-3
C₁₀H₉NO₂
Mw 175.18

**4-Fluoroindole, 97%**

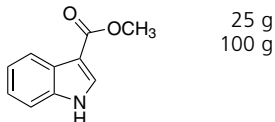
45,739-6
C₈H₆FN
Mw 135.14

**3-(Trifluoroacetyl)indole, 99%**

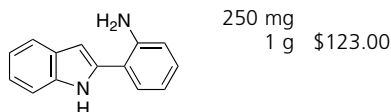
42,222-3
C₁₀H₆F₃NO
Mw 213.16

**Methyl indole-3-carboxylate, 99%**

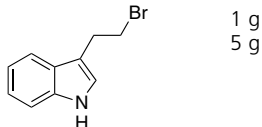
39,530-7
C₁₀H₉NO₂
Mw 175.18

**2-(2-Aminophenyl)indole, 97%**

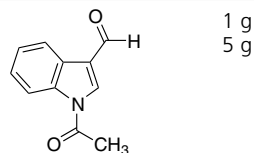
37,686-8
C₁₄H₁₂N₂
Mw 208.26

**3-(2-Bromoethyl)indole, 97%**

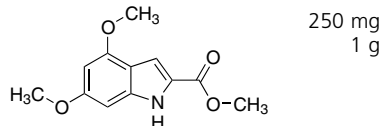
37,652-3
C₁₀H₁₀BrN
Mw 224.1

**1-Acetyl-3-indolecarboxaldehyde, 98%**

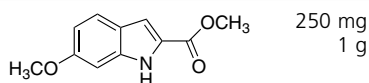
37,577-2
C₁₁H₉NO₂
Mw 187.19

**Methyl 4,6-dimethoxy-2-indolecarboxylate, 99%**

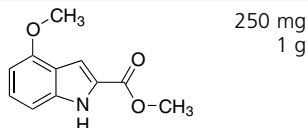
36,558-0
C₁₂H₁₃NO₄
Mw 235.24

**Methyl 6-methoxy-2-indolecarboxylate, 99%**

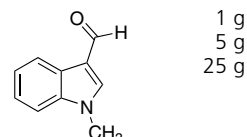
36,557-2
C₁₁H₁₁NO₃
Mw 205.21

**Methyl 4-methoxy-2-indolecarboxylate, 99%**

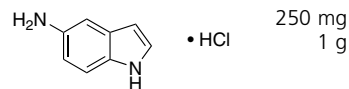
36,556-4
C₁₁H₁₁NO₃
Mw 205.21

**1-Methylindole-3-carboxaldehyde, 97%**

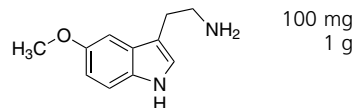
35,798-7
C₁₀H₉NO
Mw 159.18

**5-Aminoindole hydrochloride, 98%**

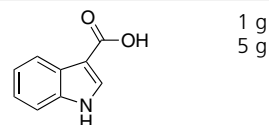
30,720-3
C₈H₈N₂ · HCl
Mw 168.62

**5-Methoxytryptamine, 97%**

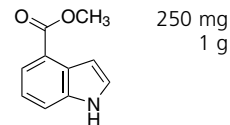
28,658-3
C₁₁H₁₄N₂O
Mw 190.24

**Indole-3-carboxylic acid, 99%**

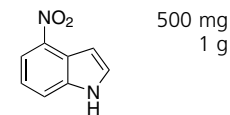
28,473-4
C₉H₇NO₂
Mw 161.16

**Methyl indole-4-carboxylate, 99%**

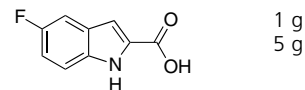
27,388-0
C₁₀H₉NO₂
Mw 175.18

**4-Nitroindole, 97%**

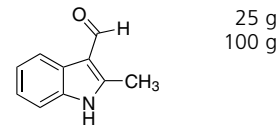
26,996-4
C₈H₆N₂O₂
Mw 162.15

**5-Fluoroindole-2-carboxylic acid, 99%**

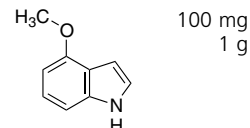
26,512-8
C₉H₆FNO₂
Mw 179.15

**2-Methylindole-3-carboxaldehyde, 97%**

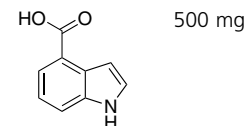
26,243-9
C₁₀H₉NO
Mw 159.18

**4-Methoxyindole, 99%**

24,629-8
C₉H₉NO
Mw 147.17

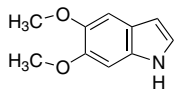
**Indole-4-carboxylic acid, 98%**

24,626-3
C₉H₇NO₂
Mw 161.16



5,6-Dimethoxyindole, 99%

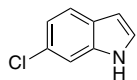
24,625-5
 $C_{10}H_{11}NO_2$
 Mw 177.2



250 mg
 1 g

6-Chloroindole, 99%

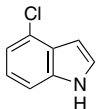
24,623-9
 C_8H_6ClN
 Mw 151.59



250 mg
 1 g

4-Chloroindole, 99%

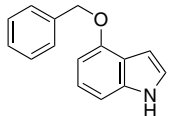
24,622-0
 C_8H_6ClN
 Mw 151.59



250 mg
 1 g

4-Benzyloxyindole, 98%

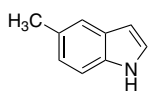
24,621-2
 $C_{15}H_{13}NO$
 Mw 223.27



1 g

5-Methylindole, 99%

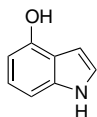
22,241-0
 C_9H_9N
 Mw 131.17



250 mg
 1 g

4-Indolol, 99%

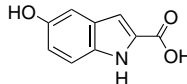
21,987-8
 C_8H_7NO
 Mw 133.15



100 mg
 250 mg
 1 g

5-Hydroxyindole-2-carboxylic acid, 98%

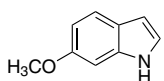
14,351-0
 $C_9H_7NO_3$
 Mw 177.16



250 mg
 1 g
 5 g

6-Methoxyindole, 98%

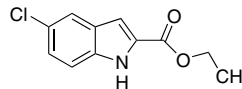
13,985-8
 C_9H_9NO
 Mw 147.17



500 mg

Ethyl 5-chloro-2-indolecarboxylate, 97%

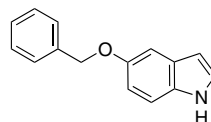
13,809-6
 $C_{11}H_{10}ClNO_2$
 Mw 223.66



5 g
 10 g

5-(Benzyloxy)indole, purum, ≥95.0% HPLC

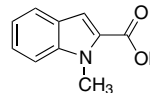
13640
 $C_{15}H_{13}NO$
 Mw 223.27



5 g
 25 g

1-Methylindole-2-carboxylic acid, 98%

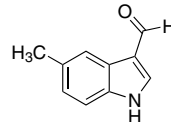
13,415-5
 $C_{10}H_9NO_2$
 Mw 175.18



1 g
 5 g

5-Methylindole-3-carboxaldehyde, 97%

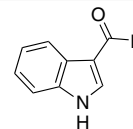
13,413-9
 $C_{10}H_9NO$
 Mw 159.18



1 g
 5 g

Indole-3-carboxaldehyde, 97%

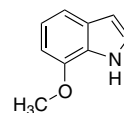
12,944-5
 C_9H_7NO
 Mw 145.16



5 g
 25 g

7-Methoxyindole, 97%

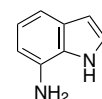
11,398-0
 C_9H_9NO
 Mw 147.17



1 g

7-Aminoindole, purum, ≥95.0% HPLC

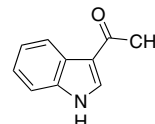
05334
 $C_8H_8N_2$
 Mw 132.16



250 mg
 1 g

3-Acetylindole, purum, ≥98.0% N

01220
 $C_{10}H_9NO$
 Mw 159.18



5 g
 25 g

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