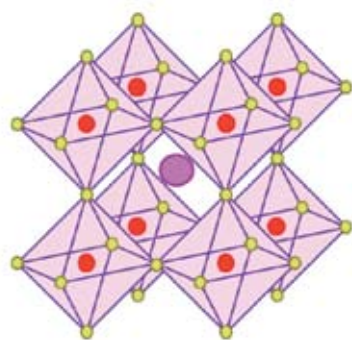


# TCIMAIL

number **164**



**Perovskite**  
**MeNH<sub>3</sub>PbI<sub>3</sub>**

## CONTENTS

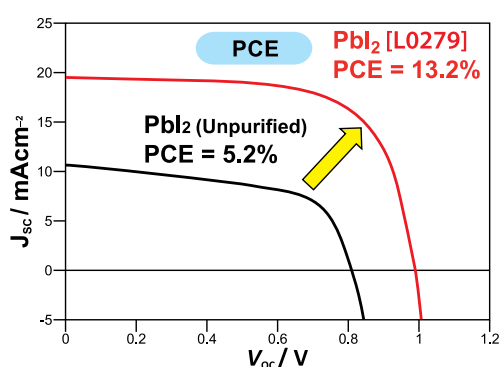
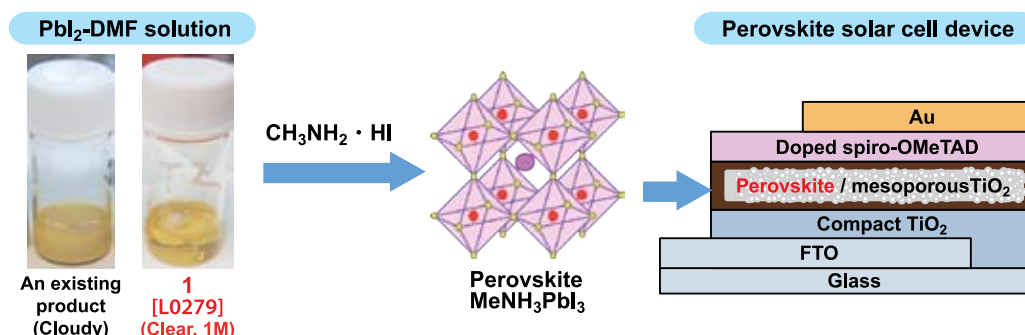
### 2 New Products Information :

- Reagent for Perovskite Solar Cells: Purified Lead(II) Iodide
- Useful Palladium Catalyst for C(sp<sup>3</sup>)-H Activation
- A New Efficient Extractant for Metal Ions Classified Soft Acids
- Symmetrical Pillar-shaped Macrocyclic Compound
- 5-hmdC: The Sixth Nucleoside of the Genome
- DRB: A Selective Inhibitor of Transcription Elongation by RNA Polymerase II
- Chemiluminescence Enhancer
- Peroxidase Detection
- Fluorescent Probe
- Glycogen Synthase Kinase (GSK) Inhibitor
- Phosphatidylinositol 3-Kinase Inhibitor

## Reagent for Perovskite Solar Cells: Purified Lead(II) Iodide

L0279 Lead(II) Iodide [for Perovskite precursor] (1)

1g, 5g



The organic-inorganic hybrid solar cell first reported in 2009 by Miyasaka *et al.*, the so-called perovskite solar cell, recently receive much attention.<sup>1)</sup> Power conversion efficiency (PCE) of the solar cell is more than 15%.<sup>2,3)</sup> A device of the perovskite solar cell can be fabricated in low cost, because it is solution-processible. At a main part of the solar cell, the organic-inorganic perovskite semiconductor ( $\text{MeNH}_3\text{PbI}_3$ ) can functionalize as an absorption layer. Wakamiya *et al.* reported that use of highly purified lead(II) iodide is a key to fabricate efficient perovskite solar cell devices (PCE > 10%) with high reproducibility.<sup>4-6)</sup> The advantages of the purified lead(II) iodide (1) are as follows: (1) it contains an extremely low quantity of water for preparing a concentrated clear DMF solution, and (2) it can fabricate perovskite solar cell devices exhibiting high PCE of more than 10%.

\*This product was produced by collaboration with Prof. Atsushi Wakamiya at Institute for Chemical Research, Kyoto University.

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A. Kojima, K. Teshima, Y. Shirai, T. Miyasaka, *J. Am. Chem. Soc.* **2009**, *131*, 6050.
- 2) Sequential deposition as a route to high-performance perovskite-sensitized solar cells  
J. Burschka, N. Pellet, S.-J. Moon, R. Humphry-Baker, P. Gao, M. K. Nazeeruddin, M. Grätzel, *Nature* **2013**, *499*, 316.
- 3) Efficient planar heterojunction perovskite solar cells by vapour deposition  
M. Liu, M. B. Johnston, H. J. Snaith, *Nature* **2013**, *501*, 395.
- 4) A. Wakamiya, M. Endo, Y. Murata, Kyoto University, JP Pat. Appl. 2014-008540.
- 5) Reproducible fabrication of efficient perovskite-based solar cells: X-ray crystallographic studies on the formation of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  layers  
A. Wakamiya, M. Endo, T. Sasamori, N. Tokitoh, Y. Ogomi, S. Hayase, Y. Murata, *Chem. Lett.* **2014**, *43*, 711.
- 6) Photocarrier recombination dynamics in perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$  for solar cell applications  
Y. Yamada, T. Nakamura, M. Endo, A. Wakamiya, Y. Kanemitsu, *J. Am. Chem. Soc.* **2014**, *136*, 11610.

### Related Products

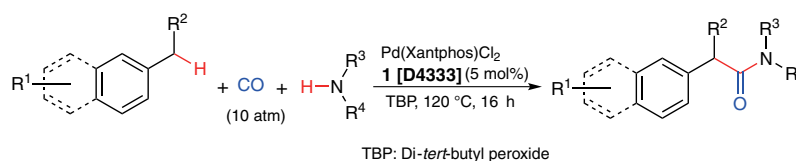
M2556	Methylamine Hydroiodide	1g	5g	25g
M2589	Methylamine Hydrobromide		1g	5g
F0974	Formamidine Hydroiodide		1g	5g
F0973	Formamidine Hydrobromide		1g	5g

Useful Palladium Catalyst for C(sp<sup>3</sup>)-H Activation

## D4333 Dichloro[9,9-dimethyl-4,5-bis(diphenylphosphino)xanthene]palladium(II) (1)

200mg, 1g

Dichloro[9,9-dimethyl-4,5-bis(diphenylphosphino)xanthene]palladium(II) (**1**) is a useful catalyst for benzylic C(sp<sup>3</sup>)-H bond activation. For example, under the presence of CO and di-*tert*-butyl peroxide (= TBP), benzylic C-H bonds of alkyl aromatics are selectively activated by the action of **1**. Subsequent aminocarbonylation with amines successfully proceeds to afford the corresponding arylacetamides.<sup>1)</sup> This reaction can be applied to substrates bearing a halogen substituent, and a subsequent cross-coupling reaction facilitates expedient synthesis of complex arylacetamides. By using this protocol, the anti-inflammatory agent ibuprofen can be easily obtained. As a similar synthetic manner, alkoxyacylations also proceed by using alcohols instead of amines.<sup>2)</sup>



Product	Yield (%)	Product	Yield (%)
	71		82
	70		67
	68		70

## Typical Procedure:

A mixture of Pd(Xantphos)Cl<sub>2</sub> (7.6 mg, 5 mol%), toluene derivative (20.0 mmol), amine (0.2 mmol) and TBP (53.0 mg, 0.36 mmol) is added into an autoclave. Then the autoclave is purged and charged with CO at 10 atm. The reaction mixture is stirred at 120 °C for 16 h, and then CO is carefully released. The corresponding reaction mixture is purified by flash column chromatography on silica gel to give the desired product.

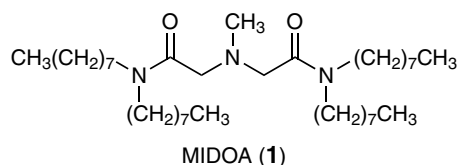
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P. Xie, C. Xia, H. Huang, *Org. Lett.* **2013**, *15*, 3370.
- 2) Palladium-catalyzed oxidative carbonylation of benzylic C-H bonds via nondirected C(sp<sup>3</sup>)-H activation  
P. Xie, Y. Xie, B. Qian, H. Zhou, C. Xia, H. Huang, *J. Am. Chem. Soc.* **2012**, *134*, 9902.

## A New Efficient Extractant for Metal Ions Classified Soft Acids

M2476 2,2'-(Methylimino)bis(*N,N*-di-*n*-octylacetamide) (= MIDOA) (1)

1mL, 5mL



2,2'-(Methylimino)bis(*N,N*-di-*n*-octylacetamide) (MIDOA or MIDAA, **1**) is a new efficient metal extractant, developed by Sasaki *et al.*<sup>1)</sup> **1** is highly lipophilic and ready to use in the HNO<sub>3</sub>(aq.)–*n*-dodecane extraction system. **1** has high extractability for metal ions classified soft acids because of the nitrogen donor atom centered in the backbones. Therefore, the distribution ratio for Tc(VII) is extremely high. In addition, Cr(VI), Re(VII), Mo(VI), W(VI), Pd(II) and Pu(IV) are well extracted by **1**.<sup>1,2)</sup>

\*This product receives a license of invention of the Japan Atomic Energy Agency (JAEA) and Ibaraki University (Japan Kokai Tokkyo Koho JP2011-001809 (2011), JP2012-144448 (2012) and Fr Pat. 2970251 (2012)).

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Y. Sasaki, Y. Kitatsuji, T. Kimura, *Chem Lett.* **2007**, *36*, 1394.
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a) Y. Sasaki, M. Ozawa, T. Kimura, K. Ohashi, *Solvent Extr. Ion Exch.* **2009**, *27*, 378. b) Y. Sasaki, Y. Sugo, M. Saeki, Y. Morita, A. Ohashi, *Solvent Extr. Res. Dev. Jpn.* **2011**, *18*, 69. c) Y. Sasaki, Y. Tsubata, Y. Kitatsuji, Y. Sugo, N. Shirasu, Y. Morita, T. Kimura, *Solvent Extr. Ion Exch.* **2013**, *31*, 401. d) M. Saeki, Y. Sasaki, A. Nakai, A. Ohashi, D. Banerjee, A. C. Scheinost, H. Foerstendorf, *Inorg. Chem.* **2012**, *51*, 5814.

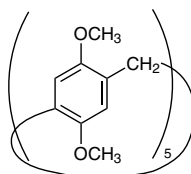
### Related Products

D4360	<i>N,N</i> -Di- <i>n</i> -octyl-3-oxapentanedioic Acid Monoamide		5g
D0504	Diethylenetriaminepentaacetic Acid (= DTPA)	25g	500g
P0811	Di(2-ethylhexyl) Phosphate (= D2EHPA)	25mL	500mL
D1585	Dibutyl <i>N,N</i> -Diethylcarbamoylmethylphosphonate	5mL	25mL
D1663	Dihexyl <i>N,N</i> -Diethylcarbamoylmethylphosphonate		5g

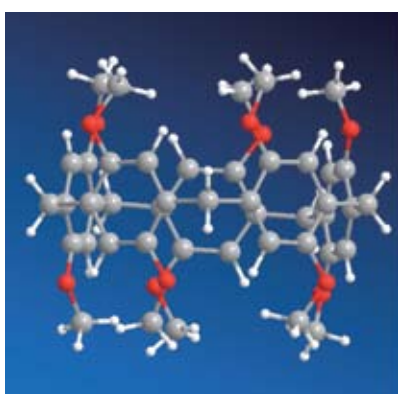
## Symmetrical Pillar-shaped Macrocyclic Compound

D4471 Dimethoxypillar[5]arene (1)

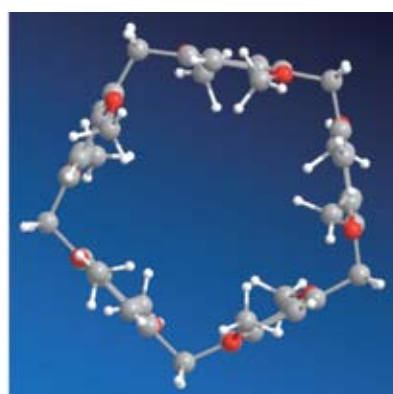
100mg



1



(a) Side View



(b) Upper View

Crystal structure of **1** from the side view (a) and the upper view (b).

Dimethoxypillar[5]arene (**1**) is a ring-shaped molecule developed by T. Ogoshi *et al.* in 2008, and has a symmetric pillar structure differing from basket-shaped calixarenes. **1** can capture electron-accepting molecules and linear *n*-alkanes selectively because the internal cavity (diameter *ca.* 0.5 nm) is an electron-rich space enclosed by benzene rings. The applications using the structural properties of **1** for host-guest chemistry and supramolecular materials such as rotaxanes are now in progress.

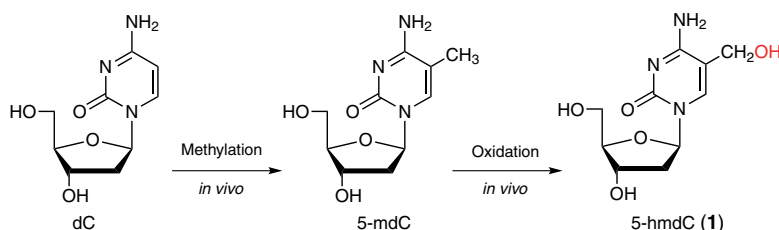
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- 3) T. Ogoshi, T. Yamagishi, *Bull. Chem. Soc. Jpn.* **2013**, *86*, 312.

## 5-hmdC : The Sixth Nucleoside of the Genome

D4220 2'-Deoxy-5-(hydroxymethyl)cytidine (= 5-hmdC) (1)

50mg, 200mg



2'-Deoxy-5-(hydroxymethyl)cytidine (5-hmdC, **1**) was recently discovered as an oxidation product of 2'-deoxy-5-methylcytidine (5-mdC) in mammalian DNA, particularly in stem cell DNA.<sup>1)</sup> The function of **1** is currently not clear, but it is assumed that in stem cells it might be an intermediate of an active demethylation process. To date the efficient detection **1** in a genome has been investigated.<sup>2)</sup>

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a) T. Pfaffeneder, B. Hackner, M. Truß, M. Münzel, M. Müller, C. A. Deiml, C. Hagemeier, T. Carell, *Angew. Chem. Int. Ed.* **2011**, *50*, 7008. b) M. Münzel, D. Globisch, T. Carell, *Angew. Chem. Int. Ed.* **2011**, *50*, 6460.
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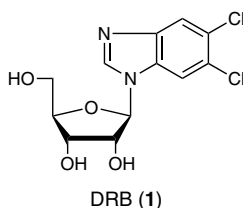
### Related Products

D3583	dC (= 2'-Deoxycytidine)	1g	5g
D3610	5-mdC (= 2'-Deoxy-5-methylcytidine)	100mg	500mg 5g

## DRB : A Selective Inhibitor of Transcription Elongation by RNA Polymerase II

D4292 5,6-Dichlorobenzimidazole 1-β-D-Ribofuranoside (= DRB) (1)

100mg, 1g



5,6-Dichlorobenzimidazole 1-β-D-ribofuranoside (DRB, **1**) is a selective inhibitor of transcription elongation by RNA polymerase II, further inhibiting mRNA synthesis in eukaryotic cells.<sup>1)</sup> The inhibition can trigger p53-dependent apoptosis of tumor cells.<sup>2)</sup> DRB can also inhibit HIV transcription by targeting elongation enhanced by the HIV-encoded transactivator (Tat).<sup>3)</sup>

### References

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L. A. Chodosh, A. Fire, M. Samuels, P. A. Sharp, *J. Biol. Chem.* **1989**, *264*, 2250.
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M. Ljungman, F. Zhang, F. Chen, A. J. Rainbow, B. C. McKay, *Oncogene* **1999**, *18*, 583.
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Y.-H. Ping, T. M. Rana, *J. Biol. Chem.* **2001**, *276*, 12951.

### Related Product

D4295	5,6-Dichlorobenzimidazole Hydrochloride	1g	5g
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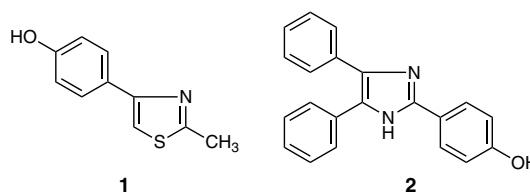
## Chemiluminescence Enhancer

M2325 4-(2-Methyl-4-thiazolyl)phenol (1)

100mg, 1g

D4178 4-(4,5-Diphenyl-1H-imidazol-2-yl)phenol (2)

100mg



Chemiluminescence has been used for analysis in life science, *e.g.* immunoassay, nucleic acid hybridization assay, Western blotting, *etc.*, as a sensitive and rapid detection method.<sup>1)</sup> Since Thorpe *et al.* reported that phenolic compounds such as 4-iodophenol enhance chemiluminescence by the peroxidase–luminol–hydrogen peroxide reaction<sup>2)</sup>, many improved methods have been reported.<sup>3)</sup> Such methods have been called enhanced chemiluminescence (ECL).<sup>3)</sup>

4-(2-Methyl-4-thiazolyl)phenol (1) and 4-(4,5-diphenyl-1H-imidazol-2-yl)phenol (2) were reported as having higher enhancing efficiency than the early type of enhancers described above.<sup>4,5)</sup>

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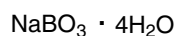
## Related Products

A5301	Luminol	1g	25g
I0840	4-Iodophenol	1g	5g
B3910	4-Bromophenol	1g	5g
S0887	Sodium Perborate Tetrahydrate	25g	500g

## Peroxidase Detection

S0887 Sodium Perborate Tetrahydrate (1)

25g, 500g

**1**

Chemiluminescence has contributed to providing high sensitivity for enzyme-linked immunoassays.<sup>1,2)</sup> Thorpe *et al.* referred that, when peroxidase is used for immunoassay as a labeled enzyme, hydrogen peroxide can be replaced by perborate.<sup>2)</sup> Compound **1** is the sodium salt of perborate. In their study,<sup>3)</sup> they used the sodium salt to replace hydrogen peroxide. **1** has already been employed for recent improvements of immunoassay.<sup>4,5)</sup>

On the other hand, interestingly, **1** has already been used as a substrate of catalase in the late 1940's.<sup>6)</sup>

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A. Tsuji, M. Maeda, H. Arakawa, *Anal. Sci.* **1989**, *5*, 497.
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G. H. G. Thorpe, L. J. Kricka, S. B. Moseley, T. P. Whitehead, *Clin. Chem.* **1985**, *31*, 1335.
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R. N. Feinstein, *J. Biol. Chem.* **1949**, *180*, 1197.



## Fluorescent Probe

F0918 FITC Dextran (Mw.=ca. 10,000) (1)

100mg

FITC dextran (fluorescein isothiocyanate-labeled dextran) is a pH-dependent lysosomal probe<sup>1,2)</sup> and has been applied to the visualization of lysosomes.<sup>3-5)</sup> FITC dextran has been used for studies on endocytic processes not only in mammal but also in yeast.<sup>6,7)</sup>

Lysosomal storage disorders (LSDs), which are defects in the lysosomal enzymes, lead to a progressive accumulation of un-degraded substrates or catabolic products that are unable to escape from the organelle.<sup>8)</sup> About 50 different clinical entities of LSDs have been genetically identified.<sup>9)</sup> Recently, the application of FITC dextran extended research for bioconjugates to target lysosomes.<sup>10)</sup>

The dextran moiety (1) is a FITC-labeled dextran with Mw. = ca. 10,000.

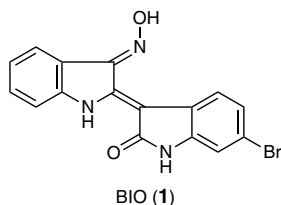
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S. Ohkuma, B. Poole, *Proc. Natl. Acad. Sci. USA* **1978**, *75*, 3327.
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S. Ohkuma, Y. Moriyama, T. Takano, *Proc. Natl. Acad. Sci. USA* **1982**, *79*, 2758.
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L. Tanasugarn, P. McNeil, G. T. Reynolds, D. L. Taylor, *J. Cell Biol.* **1984**, *98*, 717.
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## Glycogen Synthase Kinase (GSK) Inhibitor

B4006 (2'*Z*,3'*E*)-6-Bromoindirubin-3'-oxime (= BIO) (1)

5mg, 25mg



(2'*Z*,3'*E*)-6-Bromoindirubin-3'-oxime (BIO, **1**) is a cell-permeable indirubin compound and acts as an inhibitor of glycogen synthase kinase-3 (GSK-3).<sup>1,2</sup> As shown below, the inhibitory activity of **1** is highly selective to GSK-3 in comparison with other kinases.<sup>1)</sup>

Inhibition of GSK by **1** mediates the activation of the Wnt signaling pathway and sustains pluripotency in human and mouse embryonic stem (ES) cells.<sup>3)</sup> **1** is also reported to induce the differentiation of neonatal cardiomyocytes and to maintain self-renewal in human and mouse ES cells.<sup>4)</sup>

**Table 1.** Selectivity of BIO to various kinases.<sup>1)</sup>

Protein Kinase	IC50 (μm)*
GSK-3α/β	0.005
CDK1/cyclin B	0.32
CDK2/cyclin A	0.30
CDK4/cyclin D1	10
CDK5/p35	0.08
erk1	>10
erk2	>10
MAPKK	10
protein kinase C α	12
protein kinase C β1	>10
protein kinase C β2	>10
protein kinase C γ	>10
protein kinase C δ	>10
protein kinase C ε	>10
protein kinase C η	>10
protein kinase C ξ	>10
cAMP-dependent PK	>10
cGMP-dependent PK	>10
casein kinase 2	>10
insulin receptor Tyr kinase	>10

1) L. Meijer, *et al.*, *Chem. Biol.* **2003**, 1255.

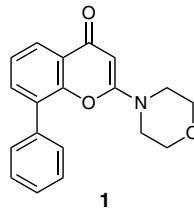
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N. Sato, L. Meijer, L. Skaltsounis, P. Greengard, A. H. Brivanlou, *Nat. Med.* **2004**, *10*, 55.
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A.-S. Tseng, F. B. Engel, M. T. Keating, *Chem. Biol.* **2006**, *13*, 957.

## Phosphatidylinositol 3-Kinase Inhibitor

M2410 LY294002 (1)

25mg



PKB/Akt, a serine/threonine kinase, regulates many kinds of important cellular functions including metabolism, proliferation, survival, apoptosis, etc.<sup>1)</sup> The kinase is activated by phosphatidylinositol 3-kinase (PI3-k) pathway.<sup>1)</sup>

LY294002 (1) is a specific inhibitor of PI3-k.<sup>2)</sup> 1 blocks the PI3-k/Akt pathway inducing apoptosis in many types of tumor cells.<sup>3)</sup> 1 also suppresses self-renewal<sup>4)</sup> and proliferation<sup>5)</sup> of embryonic stem cells and enhances the generation of mouse induced pluripotent stem (iPS) cells.<sup>6)</sup>

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B. A. Hemmings, D. F. Restuccia, *Cold Spring Harb. Perspect. Biol.* **2012**, 4, a011189.
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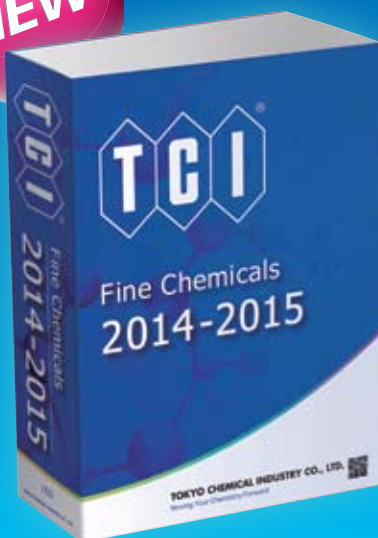
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