

# VWR® green chemicals

## Safer & sustainable alternatives

01. PREPARED  
FOR THE FUTURE

02. GREEN CHEMISTRY

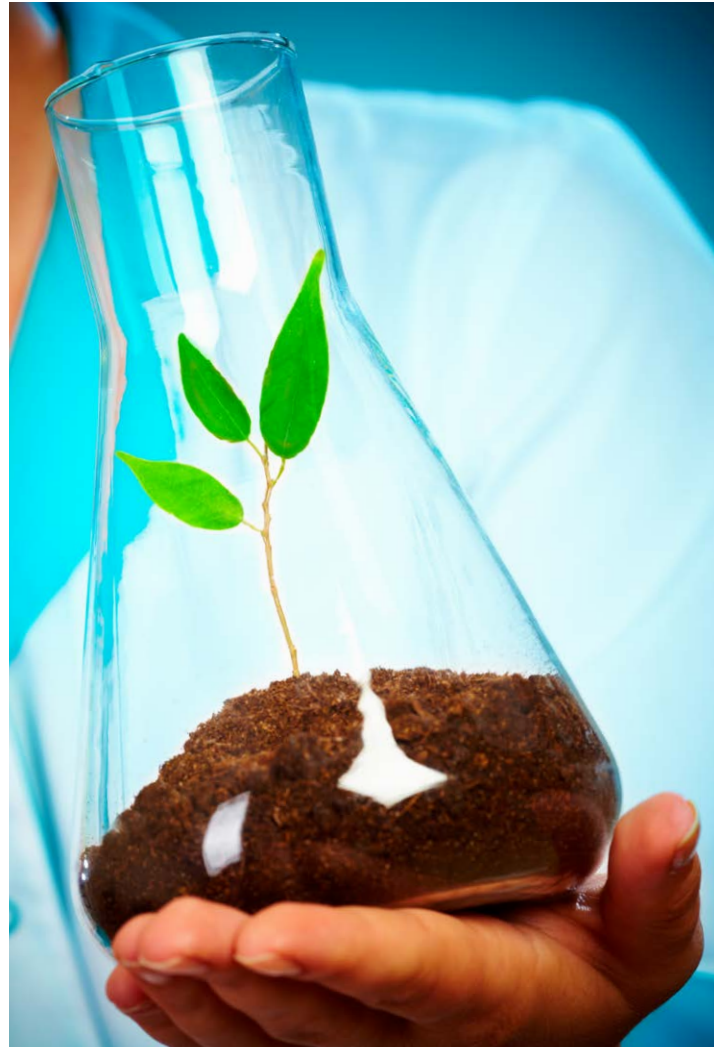
03. GREEN SOLVENTS –  
VIABLE ALTERNATIVES



# Prepared for the future

Green solvents are environmentally friendly solvents, or biosolvents which are derived from the processing of agricultural crops. The use of petrochemical solvents is the key to most chemical processes, but not without severe implications on the environment. Green solvents were developed as a more environmentally friendly alternative to petrochemical solvents.

In research laboratories and the chemical industry, organic solvents constitute the most important group of chemicals due to their huge amount of use annually. The vast majority of them are toxic and have a significant impact on human health and the environment.



In 1998, developed by Paul Anastas and John Warner, they outlined an early concept of what would make a greener chemical, process, or product.

## THE 12 PRINCIPLES OF GREEN CHEMISTRY



### PREVENTION

"It's better to prevent waste than to treat or clean up waste after it has been created." Berkeley W Cue, Ph.D., BWC PHARMA Consulting, LLC

### ATOM ECONOMY

"Synthetic methods should be designed to maximise incorporation of all materials used in the process into the final product." Michael Cann, Ph.D. Professor of Chemistry, University of Scranton

### LESS HAZARDOUS CHEMICAL SYNTHESIS

"Wherever practicable, synthetic methods should be designed to use and generate substances that possess little or no toxicity to human health or environment." David J. C. Constable, Director, ACS Green Chemistry Institute

### DESIGNING SAFER CHEMICALS

"Chemical products should be designed to preserve efficacy of function while reducing toxicity." Nicholas D Anastas, Ph.D. US, Environmental Protection Agency, New England

### SAFER SOLVENTS AND AUXILIARIES

"The use of auxiliary substances should be made unnecessary wherever possible and, innocuous when used." Dr Conception Jimenez Gonzalez, Director Operational Sustainability, Glaxo SmithKline



**DESIGN FOR ENERGY EFFICIENCY**

"Energy requirements should be recognised for their environmental and economic impacts and should be minimised. Synthetic methods should be conducted at ambient temperature and pressure." David J. C. Constable, Director, ACS Green Chemistry Institute

**USE OF RENEWABLE FEEDSTOCKS**

"A raw material or feedstock should be renewable rather than depleting whenever technically and economically practicable." Dr Richard Wool, Professor of Chemical and Biomolecular Engineering and Director of the Affordable Composites from Renewable Materials Program, University of Delaware

**REDUCE DERIVATIVES**

"Unnecessary derivatisation should be minimised or avoided if possible, because such steps require additional reagents and can generate waste." Peter J Dunn, Green Chemistry Lead, Pfizer

**CATALYSIS**

"Catalytic reagents (as selective as possible) are superior to stoichiometric reagents." Roger A Sheldon, Ph.D. Emeritus Professor of Bio Catalysis and Organic Chemistry, Delft University of Technology and CEO of CLEA Technologies B.V.

**DESIGN FOR DEGRADATION**

"Chemical products should be designed so that at the end of their function they break down into innocuous degradation products, and do not persist in the environment." Rich Williams, Founder and President at Environmental Science and Green Chemistry Consulting, LLC

**REAL TIME ANALYSIS FOR POLLUTION PREVENTION**

"Analytical methodologies need to be further developed to allow for real time, in-process monitoring and control prior to the formation of hazardous substances" Douglas Raynie, Assistant Professor, Chemistry and Biochemistry, South Dakota State University

**INHERENTLY SAFER CHEMISTRY FOR ACCIDENT PREVENTION**

"Substances and the form of a substance used in a chemical process should be chosen to minimise the potential for chemical accidents, including releases, explosions and fires." Shelly Bradley, Campus Chemical Compliance Director, Hendrix College, DR David C Finster, Professor of Chemistry, Wittenberg University, and Dr Tom Goodwin, Elbert L Fausett, Professor of Chemistry, Hendrix College

All our green solvents answer these principles and offer the following advantages:

- Less toxic and less hazardous
- Quick drying and easy to recycle
- Higher biodegradability
- Reduced chemical waste
- Higher boiling points compared to classical solvents
- Less volatile
- Reduction of solvent loss
- Contribution to reduction of energy and CO<sub>2</sub> emissions

# Our range of green solvents

Description	Cyclopentyl methyl ether GPR RECTAPUR®	2- Methyl tetrahydrofuran GPR RECTAPUR®	2- Methyl tetrahydrofuran anhydrous	1,3 Propanediol GPR RECTAPUR®	1,3 Dioxalane GPR RECTAPUR®
Cat. No. 250 ml (with septum cap)	-	-	85820.230	-	-
Cat. No. 500 ml (with septum cap)	-	-	85820.269	-	-
Cat. No. 1 L	84565.290	87132.290	-	87134.290	87135.290
Cat. No. 2,5 L	-	87132.320	-	-	-
Cat. No. 5 L	84565.360	-	-	87134.360	87135.360
Cat. No. 23/25 L	-	87132.460	-	-	87135.460
Cat. No. 200 L	-	87132.550	-	-	-
CAS No.	5614-37-9	96-47-9	96-47-9	504-63-2	646-06-0
Molecular formula	C <sub>6</sub> H <sub>12</sub> O	C <sub>5</sub> H <sub>10</sub> O	C <sub>5</sub> H <sub>10</sub> O	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>
Molecular weight	100,16 g/mol	86,13 g/mol	86,13 g/mol	76,1 g/mol	74,08 g/mol
Density	0,86 g/cm <sup>3</sup> (20 °C)	0,86 g/cm <sup>3</sup> (20 °C)	0,86 g/cm <sup>3</sup> (20 °C)	1,0597 g/cm <sup>3</sup> (20 °C)	1,066 g/cm <sup>3</sup> (20 °C)
Melting point	-140 °C	-136 °C	-136 °C	-32 °C	-95 °C
Assay on anhydrous substance	Min. 99,9%	Min. 99%	Min. 99,8%	Min. 99,7%	Min. 99,0%
Colouration	Max. 10 APHA	-	-	Max. 15 APHA	-
Formaldehydes	-	-	-	-	Max. 0,1%
Methanol	-	-	-	-	Max. 0,1%
Peroxides (as H <sub>2</sub> O <sub>2</sub> )	Max. 50 ppm	-	Max. 15 ppm	-	-
Water	Max. 100 ppm	Max. 300 ppm	Max. 30 ppm	Max. 500 ppm	Max. 500 ppm

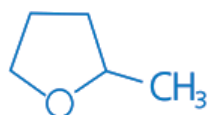
## Green solvents as alternatives to other petroleum solvents

Description	Cyclo pentyl methyl ether (CPME)	2 Methyl tetrahydrofuran (2 MeTHF)	1,3 Propanediol	1,3 Dioxalane
Dichloromethane (DCM)		✓		✓
Tetrahydrofuran (THF)	✓	✓		✓
Dimethylsulphoxide (DMSO)				✓
N,N Dimethylformamide (DMF)				
Tert butyl methyl ether (MTBE)	✓			
1,4 Dioxane	✓			
Diethyl ether	✓			
Toluene				✓
Xylene				✓
Petroleum derivates			✓	
Cat. No.	84565*	87132*	87134*	87135*

# Product specifications

## 2- METHYL TETRAHYDROFURAN (2-METHF) GPR RECTAPUR® - 87132\*

CAS NO.: 96-47-9



A real Green alternative to dichloromethane and tetrahydrofuran

This solvent, produced from natural sources (corn, sugar), combines the physical properties of THF and toluene.

### Features and benefits

- Very low toxicity
- Lower peroxide formation than THF (stabiliser required)
- Polar solvent:
  - Combines the physical properties of THF and toluene
- Can be more easily dried than THF and DCM
- Forms an azeotrope rich with water
- Excellent power of separation:
  - Limited miscibility in water (4,1 g/100 g @ +23 °C)
- Higher boiling point (80 °C) compared to THF
- Low heat vaporisation
- Can be recycled easily
- Stability in acid and caustic area
- Reduces environmental impact

### Alternative to tetrahydrofuran for organometallic reactions

- Grignard
- Reformatski
- Lithiation
- Hydride reduction
- Metal catalysed coupling

### Alternative to dichloromethane for biphasic reaction

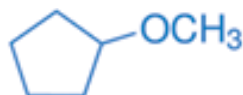
- Alkylation
- Amidation
- Nucleophilic substitution reactions

Available in **1 L** (87132.290), **2.5 L** (87132.320), **25 L** (87132.460) and **200 L** (87132.550)



## CYCLOPENTYL METHYL ETHER (CPME) GPR RECTAPUR® - 84565\*

CAS NO.: 5614-37-9



Environmentally friendly alternative to tetrahydrofuran, tert-butyl methyl ether (MTBE), 1,4 dioxane and other ether solvents.

CPME provides a green solution for those looking to improve their chemical process by, not only minimising the solvent waste stream, but also improving laboratory safety due to CPME's unique composition which resists the formation of peroxides.

### Features and benefits

- More stable than THF and 2 Me-THF
  - Resists peroxides formation
  - Narrow explosion area
- High hydrophobicity
  - Useful in many organometallic reactions
  - Provides better yields and higher selectivity over THF
- Forms an azeotrope rich with water
  - Can be more easily dried than THF or DCM
- Good power of separation
  - Limited miscibility in water (1,1 g/100 g @ +23 °C)
- Higher boiling point (106 °C) compared to THF and 2-MeTHF
- Low heat vaporisation
  - Less solvent loss during reaction reflux
  - Saves energy during distillation and recovery
- Relatively stable to acids and bases

### CPME applications

- Organic synthesis
- Grignard reaction
- Suzuki coupling
- Metal reduction
- Reaction with Lewis acids
- Friedel Crafts reactions

### And:

- Crystallisation
- Polymerisations
- Coatings
- Extractions

Available in 1 L (84565.290) and 5 L (84565.360)



**1,3 PROPANEDIOL GPR RECTAPUR® - 87134\***

CAS NO.: 504-63-2



This product is produced from a renewable source (corn). It presents very good performance, higher than a petrochemical source. Less corrosive compared to formulations from glycol or ethylene glycol. Can be viable alternative to petroleum derivatives.

**Features and benefits**

- Very low toxicity and biodegradability
- Reduces environmental impact
- Best termic stability
- Less corrosive compared to formulations from glycol or ethylene glycol

**1,3 Propanediol applications**

- Use in polyester resins
- Use in urethan chemistry
- Use as an anti-freeze or calorific transfer fluid

Available in 1 L (87134.290) and 5 L (87134.360)

**1,3 DIOXOLANE GPR RECTAPUR® - 87135\***

CAS NO.: 646-46-0



Environmentally friendly alternative to dichloromethane, dichloroethane, methyl ethyl ketone in neutral or caustic conditions.

It could be also an excellent alternative to tetrahydrofuran and DMSO in specific conditions, toluene and xylene for metallic paints.

This product can be used like a reagent or solvent.

**Features and benefits**

- No carcinogens, not toxic, not explosive, odourless and not flammable
- Produces few peroxides
- Miscible in water and the majority of solvents

**1,3 Dioxolane applications**

- Organic synthesis
- Polymer industries
- Use like a solvent in pharma
- Use for improving the dyeing texture in textile industries
- Solvent in paint and pesticide industries
- Stabilisant for halogenated solvents
- One of the components for lithium batteries
- Cleaning agent
- Use for cleaning baths

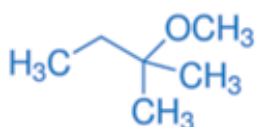
Available in 1 L (87135.290), 5 L (587135.360) and 23 L (87135.460)





## METHOXPENTANE™ GPR RECTAPUR® – 87063\*

CAS N° : 994-05-8



METHOXPENTANE™ (2-Methoxy-2-methyl butane) is a novel high quality ether solvent developed by INEOS Oligomers for demanding applications in the manufacture of high value fine chemicals, advanced life science intermediates, API's, and high-tech chemicals.

The product can be used as a versatile aprotic, halogen-free solvent in chemical synthesis and processing or as a precursor in chemical manufacturing.

METHOXPENTANE™ offers a range of unique solvent properties which helps to support user creativity in the identification of new applications for the product

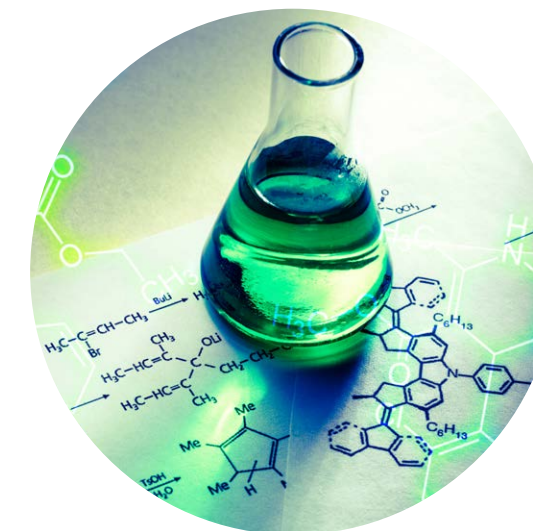
### Features and benefits

- Can be used as a versatile aprotic, halogen free in organic synthesis
- Miscible with many classical solvents (n Hexane, n Heptane, Toluene)
- Low miscibility with water interesting in organo metallic synthesis and liquid aqueous separations
- Wide application temperature range (170°) offers opportunities for use in many processing operations
- Easy to recycle with low evaporation point offering advantages in distillation and drying
- Safe due to an high flash point, no peroxides production and less toxic
- Reduce chemical waste with high biodegradability

Available in 1 L (87063.290), 5 L (87063.360) and 25 L (87063.460)

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TO LEARN  
MORE !

# Comparisons between green solvents and other solvents



Description	2 Methyl tetrahydrofuran	Cyclopentyl methyl ether (CPME)	1,3 Propanediol	1,3 Dioxalane	Methoxypentane™	N,N Dimethylformamide	N Methyl 2 pyrrolidone	Methyl ethyl ketone	Tetrahydrofuran	Diethyl ether	1,4 Dioxane	tert Butyl methyl ether (MTBE)	Dichloromethane
Cat. No.	87132*	84565*	87134*	87135*	87063*	23470*	26211*	25641*	28552*	23809*	23532*	22104*	23367*
Pk	1 L; 5 L; 25 L & 200 L	1 L & 5 L	1 L & 5 L	1 L; 5 L & 25 L	1 L; 5 L & 25 L	1 L; 2,5 L & 20 L	1 L; 2,5 L; 20 L & 204 L	1 L; 2,5 L; 5 L; 25 L & 200 L	1 L; 2,5 L; 5 L & 25 L	1 L; 2,5 L; 5 L & 25 L	1 L; 5 L; & 25 L	1 L; 2,5 L & 25 L	1 L; 2,5 L; 5 L; 25 L & 189 L
CAS	96-47-9	5614-37-9	504-63-2	646-06-6	994-05-8	68-12-2	872-50-4	78-93-3	109-99-9	60-29-7	123-91-1	1634-04-4	75-09-2
Molar mass	86,14 g/mol	100,16 g/mol	76,1 g/mol	74,08 g/mol	102,17	73,095 g/mol	99,13 g/mol	72,11 g/mol	72,108 g/mol	74,124 g/mol	88,107 g/mol	88,15 g/mol	84,93 g/mol
Density (20 °C)	0,85 g/cm <sup>3</sup>	0,86 g/cm <sup>3</sup>	1,053 g/cm <sup>3</sup>	1,067 g/cm <sup>3</sup>	0,77	0,95 g/cm <sup>3</sup>	1,03 g/cm <sup>3</sup>	0,806 g/cm <sup>3</sup>	0,89 g/cm <sup>3</sup>	0,71 g/cm <sup>3</sup>	1,03 g/cm <sup>3</sup>	0,74 g/cm <sup>3</sup>	1,36 g/cm <sup>3</sup>
Boiling point	80 °C	106 °C	214 °C	75,6 °C	85,0	153 °C	202 °C	79,6 °C	65 °C	34,6 °C	101 °C	55 °C	39,6 °C
Melting point	-136 °C	-140 °C	-27 °C	-95 °C	-80,0	-61 °C	-24 °C	-86 °C	-108,5 °C	-116,3 °C	11,8 °C	-108,7 °C	-97 °C
Flash point	-11 °C	-1 °C	129 °C	-6 °C	-7,0	58 °C	93 °C	-5 °C	-14,5 °C	-45 °C	12 °C	-28 °C	-
Viscosity (20 °C)	0,6 (25 °C) Cp	0,55 Cp	0,52 Cp	0,6 (25 °C) Cp	-	0,80 Cp	1,65 Cp	0,39 Cp	0,55 Cp	0,24 Cp	1,31 Cp	-	0,43 Cp
Vaporisation Kcal/kg	89,7 Kcal/kg	69,2 Kcal/kg	-	114 Kcal/kg	-	-	-	118 Kcal/kg	98,1 Kcal/kg	86,08 Kcal/kg	98,6 Kcal/kg	81,7 Kcal/kg	79 Kcal/kg
Refractive index (20 °C)	1,406	1,419	1,439	1,397	1,389	1,42	1,47	1,38	1,407	1,353	1,422	1,369	1,42
Dielectric constant (25 °C)	7,00	4,76	-	7,34	-	-	-	18,00	7,58	4,20	2,23	-	11,00
Azeotrop with water	71 °C	83 °C	-	71 °C	74,0	-	-	-	64 °C	34,2 °C	87,8 °C	-	-
Solubility in water 23 °C	14,00 g/100 g	1,1 g/100 g	-	-	11,5	-	-	22,6 g/100 g	-	6,5 g/100 g	-	4,8 g/100 g	1,32 g/100 g
Water solubility in solvent 23 °C	4,4 g/100 g	0,3 g/100 g	-	-	4,20	-	-	9,9 g/100 g	-	1,2 g/100 g	-	1,5 g/100 g	0,14 g/100 g
Explosion parameter vol% min. value	1,5	1,1	2,6	2,1	-	2,2	1,3	1,8	1,84	1,85	2,0	1,6	13,0
Explosion parameter vol% max. value	8,9	9,9	16,6	20,5	-	16,00	9,5	11,5	11,8	48,0	22,0	15,1	22,0

## Other potential solvent alternatives

Other potential alternative products for environmentally hazardous and harmful reagents

Description	CAS No.	Alternative to:	100 mL	500 mL	1 L	2.5 L	25 L
Anisole ≥99%, GPR RECTAPUR®	100-66-3	Chlorobenzene, Toluene	87106.180	87106.260	87106.290	87106.320	87106.460
4-Hydroxy-4-methyl-2-pentanone ≥98%, TECHNICAL	123-42-2	Acetone, chlorinated solvents			23424.290		
4-Hydroxy-4-methyl-2-pentanone ≥98%, TECHNICAL	123-42-2	Acetone, chlorinated solvents			23427.290	23427.320	23427.460
Isopropyl acetate ≥99%, GPR RECTAPUR®	108-21-4	Dichloromethane			87068.290	87068.320	87068.320
Propylene carbonate ≥99.0% (by GC), GPR RECTAPUR®	108-32-7	Acetone, N,N Dimethylformamide, chlorinated solvents			87076.290		87076.460

# Bio-based solvents

## Advantages:

- Non-synthetically manufactured ethanol
- Low toxicity during the production processes
- No dependant of the petroleum cost prices

For some classical solvents, our objective is also to implement sustainable initiatives. For instance, we've decided to change from solvents based on synthetic chemicals to those from renewable raw materials. If possible, we will choose chemical products which preserve functional efficacy while reducing toxicity and environmental impact, also in the production processes safer for the environment than with fossil-based solvents..

## Features and benefits

- All alcohols (20821\* and 20816\*) are produced from yeast fermentation of agricultural substrates (beets or wheat)
- All denatured Ethanols (85829\*, 85830\*, 85824\*, 85823\*, 85828 and 85825\*) are produced from natural origin (wheat, corn, sugar cane)
- All Glycerines are produced from vegetable origin

Description	CAS No.	1 L (GB)	1 L (PB)	2.5 L (GB)	2.5 L (PB)	5 L (PB)	10 L (PB)	20 L (PB)	25 L
Ethanol absolute ≥99.8%, AnalaR NORMAPUR® ACS, Reag. Ph. Eur. analytical reagent	64-17-5	20821.296	20821.310	20821.321	20821.330	20821.365			20821.467
Ethanol absolute ≥99.5%, GPR RECTAPUR®	64-17-5					20820.362			20820.464
Ethanol 96% (v/v), AnalaR NORMAPUR® analytical reagent	64-17-5	20823.293		20823.327		20823.362			20823.460
Ethanol, GPR RECTAPUR®	64-17-5		20824.296		20824.321	20824.365			20824.467
Ethanol absolute ≥99.5% Ph. Eur., USP	64-17-5	20816.298				20816.367			20816.470
Ethanol ≥96% Ph. Eur.	64-17-5	20905.296		20905.320		20905.365			20905.467
Ethanol Eurodenatured ≥96%, GPR RECTAPUR® (1:1:1)	64-17-5		85829.290		85829.320	85829.360	85829.410		85829.460
Ethanol Eurodenatured ≥99%, GPR RECTAPUR® (1:1:1)	64-17-5		85830.290		85830.320	85830.360	85830.410		85830.460
Ethanol Eurodenatured ≥96%, TechniSolv® (1:1:1)	64-17-5					85824.360	85824.410	85824.440	
Ethanol Eurodenatured ≥99%, TechniSolv® (1:1:1)	64-17-5					85823.360	85823.410	85823.440	
Ethanol Eurodenatured ≥80%, TechniSolv® (1:1:1)	64-17-5							85828.440	
Ethanol Eurodenatured ≥70%, TechniSolv® (1:1:1)	64-17-5							85825.440	
Glycerine ≥99.5%, AnalaR NORMAPUR® ACS analytical reagent, redistilled	56-81-5	24388.295		24388.320		24388.364		24388.444	
Glycerine 86%, AnalaR NORMAPUR® analytical reagent	56-81-5	24385.295		24385.320					24385.460
Glycerine (glycerol) Ph. Eur., USP, BP	56-81-5	24386.298				24386.367			
Glycerol ~86% Ph.Eur., extra pure	56-81-5	24384.290		24384.320					24384.460

PB = Plastic bottle  
GB = Glass bottle

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# Setting science in motion to create a better world



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