

Biotage PathFinder™



www.biotagepathfinder.com

Access thousands of microwave reactions through a single database

Biotage PathFinder Web is the world's largest online database of established methods for microwave synthesis. The new web-based format offers chemists worldwide access to more than 3800 diverse microwave methods. Using a simple keyword and/or substructure search, it is fast and easy to find microwave conditions for your reactions, along with experimental details. Monthly updates are contributed from scientific partners and recent literature. Reactions are checked for accuracy and ambiguous processes are verified with authors directly, a level of cross-checking unique to the PathFinder.

PathFinder Data

Coverage: 2000 – present

Focus: Microwave synthesis with explicit experimental details

Source: Approximately 70% Biotage internal unpublished results; 15% contributions from scientific partners; 15% published data

Size: more than 3,800 reactions

Updates: Monthly, online

Biotage PathFinder Web Subscription will provide you with:

- **Low cost** annual access to a growing database of microwave reactions
- **Suitable conditions** and **starting points** for a variety of microwave assisted reactions
- Access to **unpublished microwave transformations**
- **Full documentation** on substrates, solvents, reagents and catalysts with quantities, experimental procedure including workup details and analytical data
- **Monthly updates** of contents with new diverse microwave reactions

PathFinder Cookbook

The cookbook will provide you a FREE taste of the microwave reactions in Biotage PathFinder. Select from a list of reaction examples for a sampling.

Examples of Reactions

- Suzuki Coupling
- Heck Coupling
- Wittig Olefin synthesis
- Amidation
- Reductive Amination
- Reduction
- Oxidation
- Nucleophilic Aromatic Substitution
- Multicomponent reactions
- Arbuzov Reaction
- Knoevenagel Condensation... and more...

PathFinder Cookbook - reaction details
Reaction id: 0210091013_18, verified by Personal Chemistry ©

Yield: 90% Time: 1500s Temperature: 180 °C

Chemicals				
Name	MW [g/mol]	Density [g/ml]	Amount [mmol]	Mass / Volume
7570458	223.275	1.000	0.500	111.637 mg
105566	113.116	1.063	0.600	63.847 µl
Piperidine (0.5M in THF)	85.150	1.000	0.100	200.000 µl
Acetic acid (0.5M in THF)	60.052	1.000	0.100	200.000 µl
EtOH	46.069	1.000	45.594	2100.000 µl
Product 1	318.376	1.000	0.500	159.189 mg

Additional Features

Ask-a-Chemist

This feature allows chemists to get quick answers to their questions directly from a Biotage chemist experienced in microwave synthesis.

Vapor-Pressure Calculator

This feature rapidly calculates the vapor pressure for commonly used solvents at different temperatures.

Prediction Chart and Time Converter

A tool to help chemists estimate the temperature required to run a microwave reaction in a shorter period of time based on conventional temperature and time.

To experience the benefits first hand, take a **Guided Tour** on our Web site,
www.biotagepathfinder.com

The screenshot displays the Biotage PathFinder web application. The interface includes a sidebar with navigation links: Home, Guided Tour, PathFinder Cookbook, Submit, Utilities, and Support. The main content area shows 'Report - reaction details' for Reaction ID: 0201111010_28, verified by Personal Chemistry. It features a chemical reaction scheme involving 1-(2-aminodethyl)boronic acid, ethyl isocyanate, and methanol (MeOH) to form a product. Below the reaction, it specifies 'Yield: 100% Time: 240s Temperature: 120 °C'. A table lists chemicals with columns for Name, MW [g/mol], Density [g/ml], Amount [mmol], and Mass/Volume. The table includes entries for 1-(2-aminodethyl)boronic acid, ethyl isocyanate, methanol, and the product. Keywords include 'Boronic Acid Mannich Reaction, Multicomponent'. Comments discuss synthesis conditions and purification. Instrument settings for absorption level and pre-stirring time are provided. References cite Petasis, N. A.; Zavialov, I. A. J. Am. Chem. Soc. 1997, 119, 445-446. An analysis table shows the method (crude LCMS, 1H NMR), purity (100), and files. The footer contains copyright information (© Biotage 2004) and links for License & Access terms, Privacy, Requirements, and Password Retrieval.

Ordering Information

Item

Biotage PathFinder

Description

Web-based database of microwave assisted synthesis reactions, single seat, annual subscription

Part Number

355239

Please contact your local Biotage representative for more information.

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