

反応回答の解析・絞り込み (Analyze/Refine)

- 反応検索によって得られた反応の回答集合に対して、12 種のデータに基づく解析 (Analyze) や 6 種の観点で絞り込み (Refine) ができます。

The screenshot shows the 'REACTIONS' interface with a reaction between a chlorinated heterocycle and a boronic acid derivative. The 'Analyze' and 'Refine' tabs are highlighted. The 'Analyze by:' dropdown is set to 'Solvent', showing a list of solvents with their respective counts.

| Solvent | Count |
|--------------------------------------|-------|
| H ₂ O | 1524 |
| THF | 1287 |
| PhMe | 875 |
| DMF | 814 |
| CH ₂ Cl ₂ | 495 |
| (CH ₃ O) ₂ | 478 |
| Dioxane | 460 |
| EtOH | 355 |
| Me(CH ₂) _n Me | 344 |
| AcNMe ₃ | 324 |

解析機能

絞り込み検索

The 'Analyze' tab shows a list of catalysts with their counts. A 'Show More' button is circled in red.

| Catalyst | Count |
|--|-------|
| Pd(PPh ₃) ₄ | 680 |
| PdCl ₂ (PPh ₃) ₂ | 177 |
| Pd(OAc) ₂ | 108 |
| Pd ₂ (dba) ₃ | 99 |
| CuI | 86 |
| 131274-22-1 | 60 |
| PPh ₃ | 48 |
| 95464-05-4 | 37 |
| 53199-31-8 | 31 |
| 4-DMAP | 27 |

クリックすると観点を選擇できる

Reagent
Author Name
Catalyst
Company-Organization
Document Type
Experimental Procedure
Journal Name
Language
Number of Steps
Product Yield
Publication Year
Reagent
Solvent

クリックして
解析の詳細表示

The 'Refine' tab shows options to filter results based on reaction structure, yield, number of steps, classification, and functional groups. A 'Structure Editor' is also visible.

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Structure Editor: Java Non-Java

Click image to change structure or view detail.
Search type: Substructure

反応式

収率

反応ステップ数

反応分類

反応に関与しない官能基

クリックして
反応作図

Refine

・解析対象データは最大 20,000 回答

