

# Solid-Phase Reaction Searching

This module teaches basic strategies for searching the SPORE database. The SPORE database contains structures and data for reactions that use solid-phase methodology. These reactions are selected from over 100 primary chemistry journals from 1963 onward. This module uses the Reaction Browser application.

## Course Objectives

The participant will be able to:

- ◆ Search for reactions using specialized solid phase reaction data fields
- ◆ Search for reactions using molecule or reaction substructures
- ◆ Use specialized browsing forms and viewing options to display relevant reaction data
- ◆ Cluster reactions on various criteria to organize and refine search results
- ◆ Combine, edit, and print search results

## Prerequisites

Reaction Searching  
Drawing Molecules

## Course Length

1/2 day

## Examples from the Class

*Searching for solid supports that could be used for Suzuki-type coupling reactions*

<b>Reaction Type</b>	<input %suzuki="" coupling%\""="" type="text" value="like \"/>
<b>Reaction Conditions</b>	<input bases\""="" organic="" type="text" value='\"%Weak'/>
<b>Ligand Linkage Stability</b>	<input type="text" value='\"%stable\""/'/>

*Clustering search results by solid support*

No.	Reactant Grade
1	24.0 - 40.0

Step	Hours	Temp C	Reflux?	pH
1	24.0 - 40.0		yes	

No.	Literature Reference
1	JACKES, B. J.; ELLMAN, J. A.; J Am Chem Soc [JACSAT] 1994, 116 (24), 11171-11172.

Cluster #	Size	Value
1	(13)	PSOX1200
2	(10)	AHBX1205
3	(9)	PSOX2400
4	(7)	PSNX1802
5	(7)	PSOX1300
6	(7)	EMOX1801
7	(5)	PSNA1200
8	(4)	PSNA2400
9	(3)	EMNA1810

*Viewing details of solid support data*

S.S. ID:	Ref.	Note(s) for solid support	Reference(s) for note
6987002		TFA-labile resin (cleaved with 50% TFA/CH <sub>2</sub> Cl <sub>2</sub> in the original report).	RINK, H.; Tetrahedron Lett [TELEAY] 1987, 28 (33), 3787-3790.
6987002		Fmoc derivative as convenient	RINK, H.; Tetrahedron Lett [TELEAY]

Pol. ID:	Ref.	Note(s) for Polymer	Reference(s) for note
6963001		Merrifield's original solid support; cleavage of the ester linkage by basic hydrolysis, ammonolysis or	MERRIFIELD, R. B.; J Am Chem Soc [JACSAT] 1963, 85, 2149-2154.

Step	Conditions	Ligand linkage	Ligand status	Polymer linkage	Polymer status
1	Small Nucleophiles Transition Metal Complexes Thermal	amide	stable	ether, benzylic, aromatic	stable