

National Chemical Database Service

@ cds.rsc.org

Properties and Reactions of Organic Systems Workshop

SPRESIweb

spresi.cds.rsc.org

[SPRESIweb](http://spresi.cds.rsc.org) is the online interface to the SPRESI structure and reaction database of:

- 5.62 million compounds
- 4.34 million reactions

ChemSpider

chemspider.com

[ChemSpider](http://chemspider.com) is an online chemical structure database of over 29 million structures from more than 440 data sources. ChemSpider builds on the collected sources by adding additional properties and data, and links back to original data sources. There are 300,000 spectra accessible via ChemSpider.

Chemicalize

cds.rsc.org/chemicalize.asp

[Chemicalize](http://cds.rsc.org/chemicalize.asp) is a public web resource which identifies chemical structures in webpages, pdf files and other text using ChemAxon's Name to Structure parsing and indicates their prevalence. Chemicalize also make structure-based predictions.

An electronic version of this workshop material can be found at <http://rsc.li/19YOBXe>

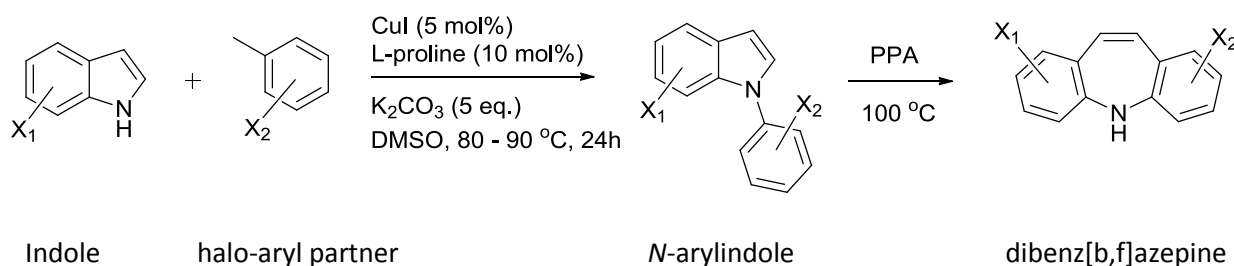
Exploring organic reactions – SPRESIweb

[“Convenient syntheses of halo-dibenz\[b,f\]azepines and carbamazepine analogues via N-arylindoles”](#)

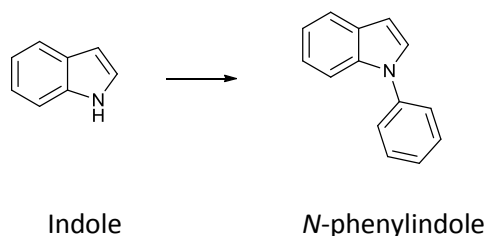
Org. Biomol. Chem., 2013, 11, 8426-8434

DOI: 10.1039/C3OB41252K

This paper details the coupling of various substituted indoles with halo-aryl partners. The *N*-arylindoles formed can be catalysed by acid to form dibenz[b,f]azepines.



For the simplest *N*-arylindole, *N*-phenylindole, how many synthetic routes from indole are present in SPRESIweb?



- Go to spresi.cds.rsc.org
- Search > Reactions **Reactions**
- Click the draw button
- **Draw the reaction** and click “Transfer”
- Change “All-In-One Reaction Search” to “**Exact Reaction**”
- Click “Search”

Reactions found:

How many of those synthetic routes are over 90% yield?

- Go back
- In the top box, select “Yield” and in the adjacent dropdown menu “>” and type “90”

Yield > 90

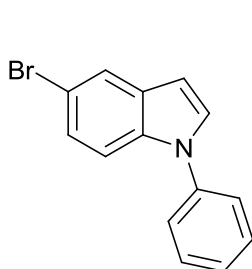
- Click “Include Reaction” INCLUDE REACTION

- Change “All-In-One Reaction Search” to “Exact Reaction” and Exact Reaction

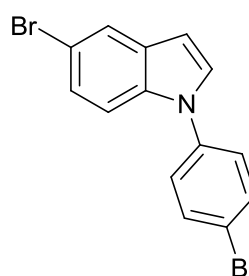
- Click “Search”

Reactions > 90% yield found:

The paper synthesises a mixture of novel and previously explored compounds. For instance **39** has been synthesised previously, but **40** has not.



39
83% yield



40
51% yield

Who has synthesised the product **39** before, and in what yield?

- Search > Molecules

- Click draw button

- Draw the structure of **39** and click “Transfer”

- Change “All-In-One Structure Search” to “Exact Structure” and Exact Structure

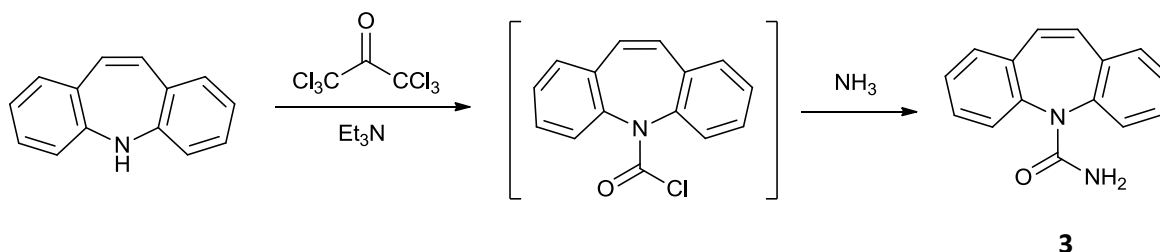
- Click “Journal Articles”

- Open the article by clicking the DOI and find the yield of the **39** synthesis reaction


Previous yield of **39** synthesis:

Exploring pharmacology – Chemicalize / ChemSpider

Dibenzazepines undergo carboxamidation with triphosgene to give molecules such as **3**.



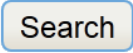
What are the pharmacological properties (effects on the body) of molecule **3**?

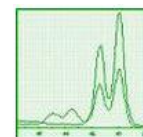
- Go to cds.rsc.org/chemicalize.asp
- Edit the structure 
- Draw **3**, click OK
- Click “**Calculate**”
- You can pick the property panel layout according to your background:
Synthetic or **Medicinal** chemist

Does molecule **3** satisfy Lipinski’s rule of five, and those of bioavailability?

- Find the “**Lipinski-like filters**” panel

Investigate the spectra associated with molecule **3**

- Copy the SMILES or InChI from Chemicalize
- Go to www.chemspider.com
- Paste the SMILES or InChI into ChemSpider
- Click “**Search**” 
- Find the “**Spectra**” panel, and click on the green icon to load the spectra



Has molecule **3** been used in any drugs?

- Find the “**Pharmacological Links**” drop down tab

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 Drug names