

Beilstein

Dialog

Beilstein on Dialog provides critical organic chemistry data in three files: Beilstein Facts (File 390), Beilstein Reactions (File 391) and Beilstein Abstracts (File 393). Use all three Beilstein files to retrieve full comprehensive information about an organic compound.

This example illustrates how to retrieve a substance record in the Facts file; get the preparation and reactions from the Reactions file; and, finally, retrieve the abstract of the data reference from the Abstracts file. For more information about the MAP command, see the Dialog Pocket Guide, available from <http://support.dialog.com/searchaids/dialog>.

File 390:BEILSTEIN FACTS

```
      Set  Items  Description
      ---  -
?s na=aspirin

      S1      1  NA=ASPIRIN
```

SELECT a substance by Name in the NA= index. For a more complicated name, start with EXPAND NA=.

?t s1/2

TYPE the record in Format 2 to see identification info and data preset. Use Format 2,GS to see the structure.

1/2/1

DIALOG(R)File 390:BEILSTEIN FACTS
All rts. reserv.

779271

This is the Beilstein Registry Number used to map to the Beilstein Reactions file.

2-acetoxy-benzoic acid

Synonym: 2-acetoxy-benzoic acid; 2-Acetoxy-benzoic acid; acetylsalicylic acid; salicylic acid acetate; 2-(acetyloxy)-benzoic acid; O-acetyl-salicylic acid; *aspirin*

CAS RN: 50-78-2*

Beilstein Cit: 0-10-00-00067 1-10-00-00028 2-10-00-00041 3-10-00-00102

(...record abbreviated...)

?map bnmain t

MAP the main Beilstein Registry number.

1 Select Statement(s), 1 Search Term(s)

Serial#TC363

1 SearchSaves, 1 Search Term(s)

?B 391

BEGIN the Beilstein Reactions file and execute the MAP command.

File 391:BEILSTEIN REACTIONS

```
      Set  Items  Description
      ---  -
?exs tc363
      S1      6  BN=779271
?s s1/product
      S2      1  S1/PRODUCT
?t s2/9
```

Limit the set you created (s1) to Aspirin as a product.

2/9/1

DIALOG(R)File 391:BEILSTEIN REACTIONS
08/17/04. All rts. reserv.

Reaction Id: 9348603

Reactants

BN=9388496 2-thioacetoxy-benzoic acid

Products

BN=*779271* 2-acetoxy-benzoic acid

No. of Reaction Details: 1

Reaction Details

Classification: Preparation

Yield: 58 percent (BN=779271)

Reagent: oxone

Time: 35 min (Ref. 1)

(...record abbreviated...)

?s s1/reactant

S3 5 S1/REACTANT

?t s3/9

3/9/1

DIALOG(R)File 391:BEILSTEIN REACTIONS

08/17/04. All rts. reserv.

Reaction Id: 9342977

Reactants

BN=2103321 N - tert -butoxycarbonyl-glycine chloromethyl ester

BN=*779271* 2-acetoxy-benzoic acid

Products

BN=9422340 2-acetoxy-benzoic acid tert
-butoxycarbonylaminoacetoxymethyl ester

No. of Reaction Details: 1

References

1, 6398304 Gomes, Paula ; Santos, Maria Isabel ; Trigo, Maria Joaquina

(...record abbreviated...)

?map ba t s3/1

1 Select Statement(s), 1 Search Term(s)

Serial#TC365

1 SearchSaves, 1 Search Term(s)

?b 393

Set	Items	Description
---	----	-----

?exs

Executing TC365

S1 1 BA=6398304

?t s1/9

1/9/1

DIALOG(R)File 393:Beilstein Abstracts

Jan. 2004. All rts. reserv.

Beilstein Abstract Id: *6398304*

Title: Improved Synthesis of Amino Acid and Dipeptide Chloromethyl Esters
Using Bromochloromethane

Document Type: Journal

Author: Gomes, Paula; Santos, Maria Isabel; Trigo, Maria Joaquina;
Castanheiro, Raquel; Moreira, Rui

Citation: Synth.Commun. (2003) Series: 33-10, 1683 - 1694 CODEN: SYNCAV
Language: English

Abstract: Peptide chloromethyl esters are important compounds in prodrug(....)

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Limit the set you created (s1) to Aspirin as a reactant.

This is the Beilstein Abstract Number used to MAP to the Abstract database.

Now, MAP the Beilstein Abstract Number for Set 3, the first record.

BEGIN Beilstein Abstracts and execute the saved search.