SciFinder
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BÚSQUEDA POR REACCIONES

Universidad Complutense Madrid

UCM BIBLIOTECA COMPLUTENSE

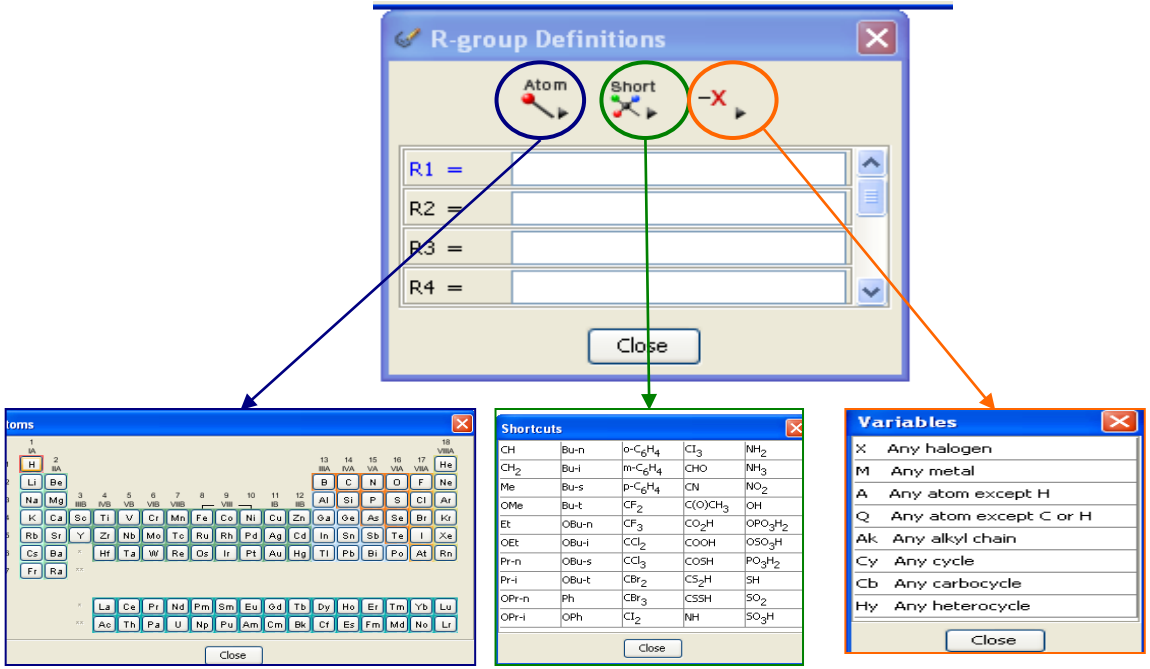
EDITOR DE DIBUJO I

Lápiz

Borrador

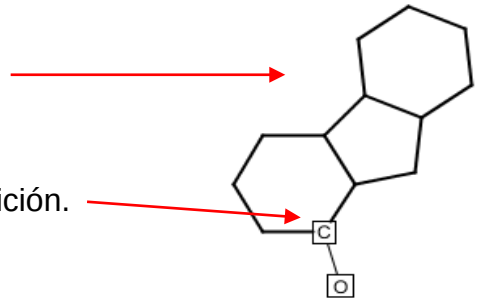
Contiene símbolos predeterminados

Contiene grupos predeterminados



EDITOR DE DIBUJO III

Para “bloquear” anillos o cadenas y que no se produzcan fusiones



Para “bloquear” átomos. Los *“shortcuts”* están bloqueados por definición.

Se usa para rotar una estructura o un fragmento – que no esté unido- en el sentido de las agujas del reloj o el contrario.

Invertir una estructura, bien horizontal o verticalmente. Se seleccionan los puntos que se quieren invertir: control + click y: a) horizontal: marcar H; b) vertical: marcar: V

Añadir carga positiva

Añadir carga positiva

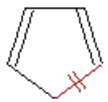
Herramientas para la búsqueda por reacciones

Flecha de reacción

La misma función que la anterior pero se despliega un cuadro de diálogo para preguntar sobre la función de la estructura o el grupo funcional en la reacción: product, reactant, reagent, **Reactant or Reagent** , cualquier función, non reacting (sólo para grupos funcionales)

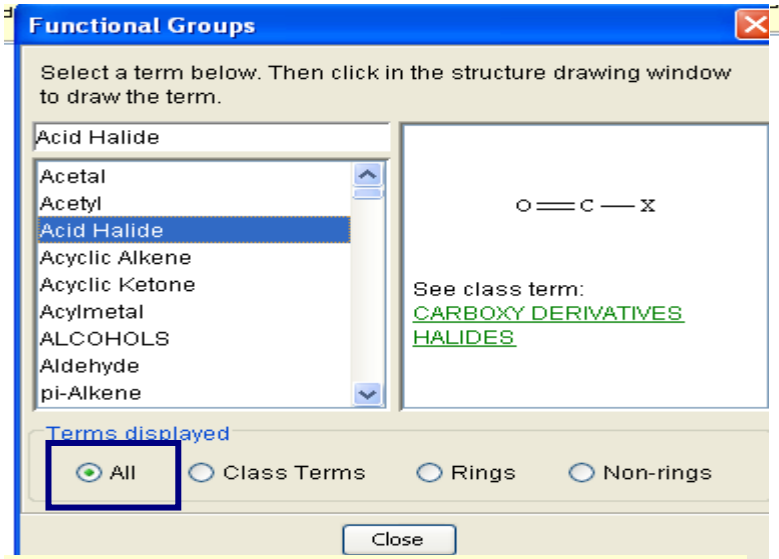
Se define un react/product o un par de átomos react/product

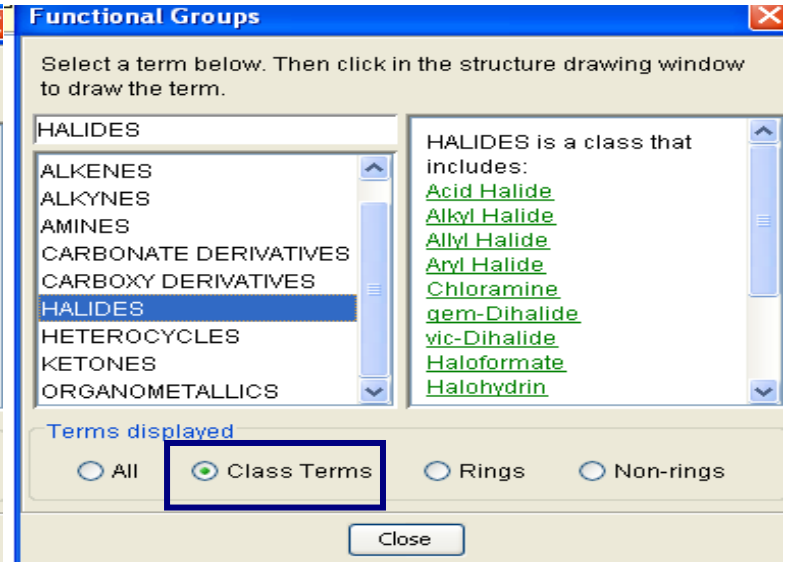
Se señala el enlace o enlaces por donde va a tener lugar una transformación

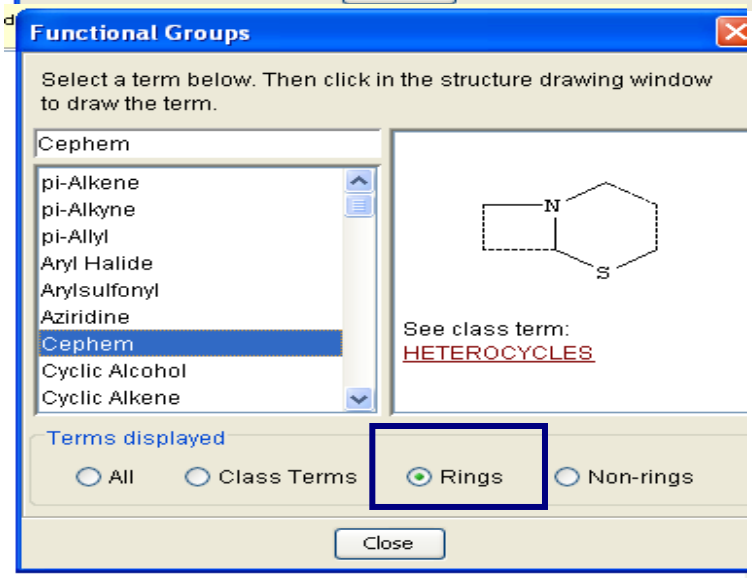


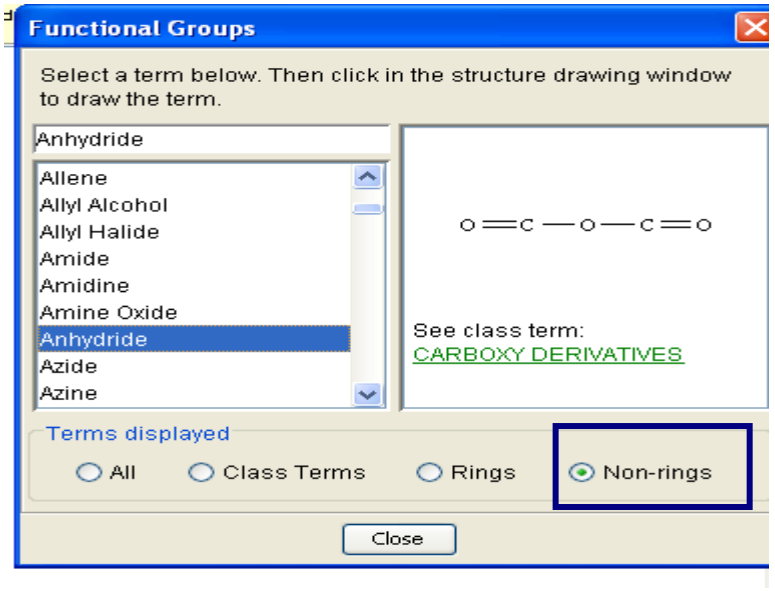
alchc
ketor
alder

Grupos funcionales









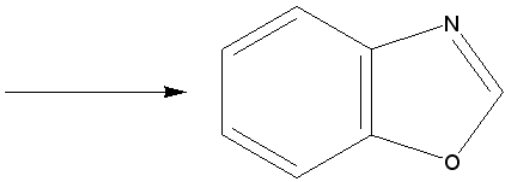
EXPLORE REACTIONS

¿Qué vamos a hacer?

1. **Una búsqueda por reacciones empleando una subestructura como producto**
2. **Refinar la búsqueda**
3. **Recuperar reacciones y eliminar las no deseadas**
4. **Recuperar las referencias en las que aparecen estas reacciones**

EJEMPLO:

Sintetización de derivados de benzoxazol (C_7H_5NO) a través de la formación de un anillo de benceno



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NEW My Connections | Prefi

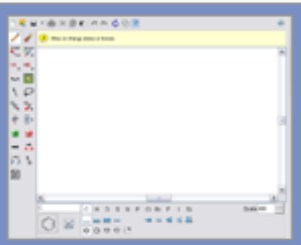
Sign Ou

Iniciaremos la búsqueda seleccionando *"Explore Reactions"*

Explore Reactions

Reaction Structure

Reaction Structure



Click image to draw or import structure

Search

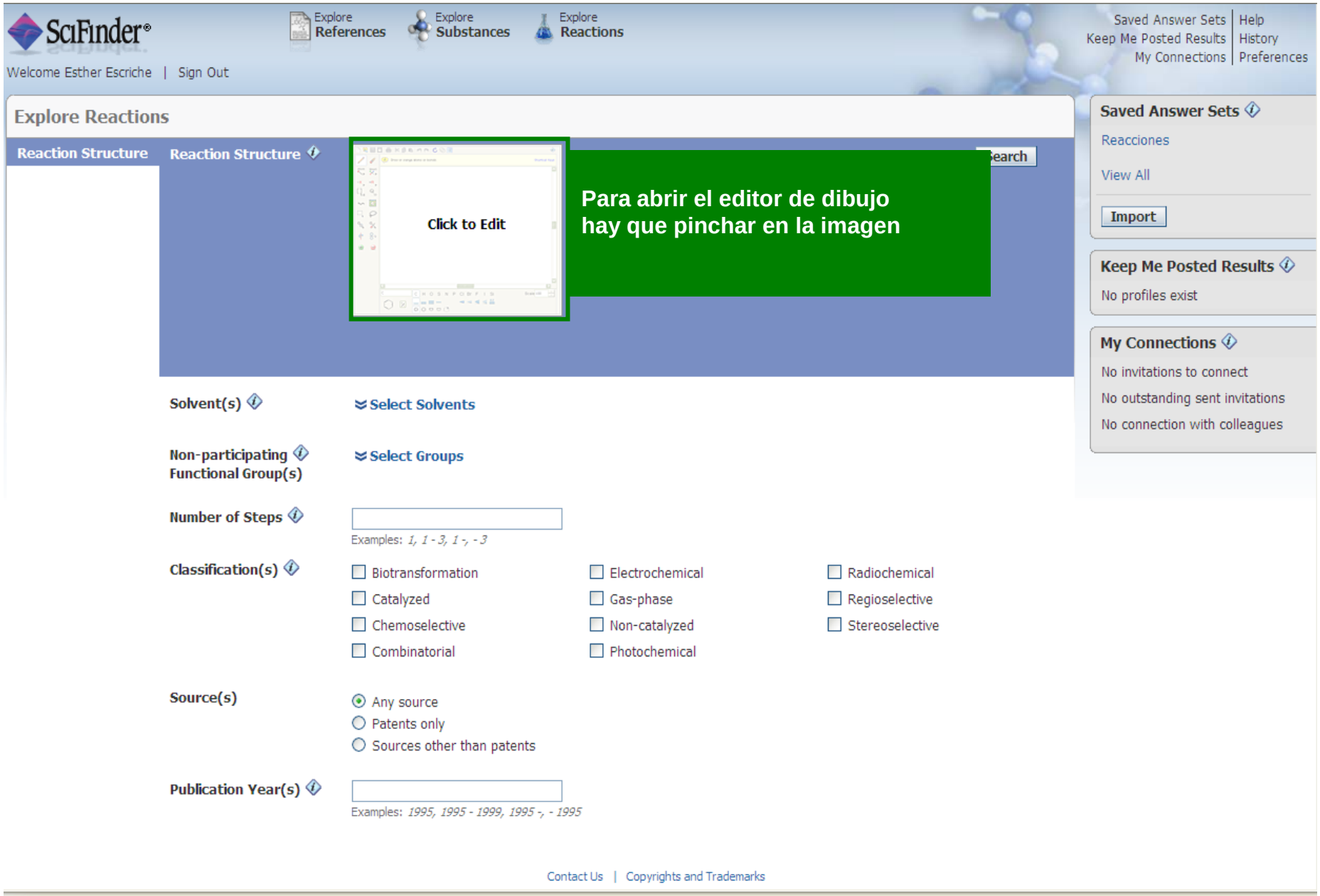
Solvents — Select Solvents NEW

Number of Steps

Examples: *1, 1 - 3, 1 -, - 3*

Classification(s)

- ☐ Biotransformation
- ☐ Catalyzed
- ☐ Chemoselective
- ☐ Combinatorial
- ☐ Electrochemical
- ☐ Gas-phase
- ☐ Non-catalyzed
- ☐ Photochemical
- ☐ Radiochemical
- ☐ Regioselective
- ☐ Stereoselective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Explore References
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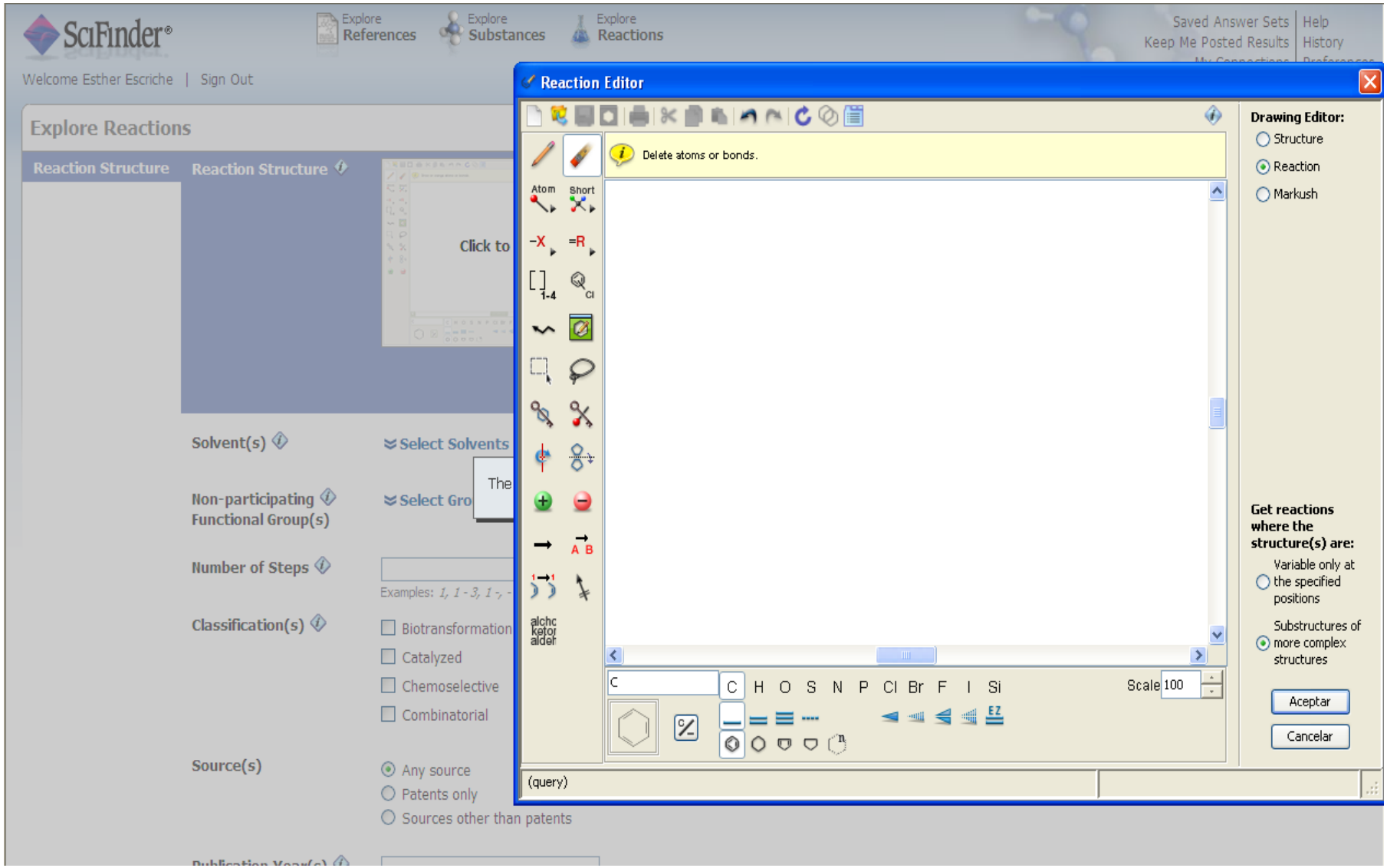
Explore Reactions
Saved Answer Sets | Help
Keep Me Posted Results | History
My Connections | Preferences
Welcome Esther Escriche | Sign Out
Explore Reactions
Reaction Structure
Reaction Structure
Click to Edit
Para abrir el editor de dibujo hay que pinchar en la imagen
Saved Answer Sets
Reacciones
View All
Import
Keep Me Posted Results
No profiles exist
My Connections
No invitations to connect
No outstanding sent invitations
No connection with colleagues
Solvent(s)
Select Solvents
Non-participating Functional Group(s)
Select Groups
Number of Steps
Examples: 1, 1 - 3, 1 -, - 3
Classification(s)
Biotransformation
Catalyzed
Chemoselective
Combinatorial
Electrochemical
Gas-phase
Non-catalyzed
Photochemical
Radiochemical
Regioselective
Stereoselective
Source(s)
Any source
Patents only
Sources other than patents
Publication Year(s)
Examples: 1995, 1995 - 1999, 1995 -, - 1995
Contact Us | Copyrights and Trademarks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Explore Reactions
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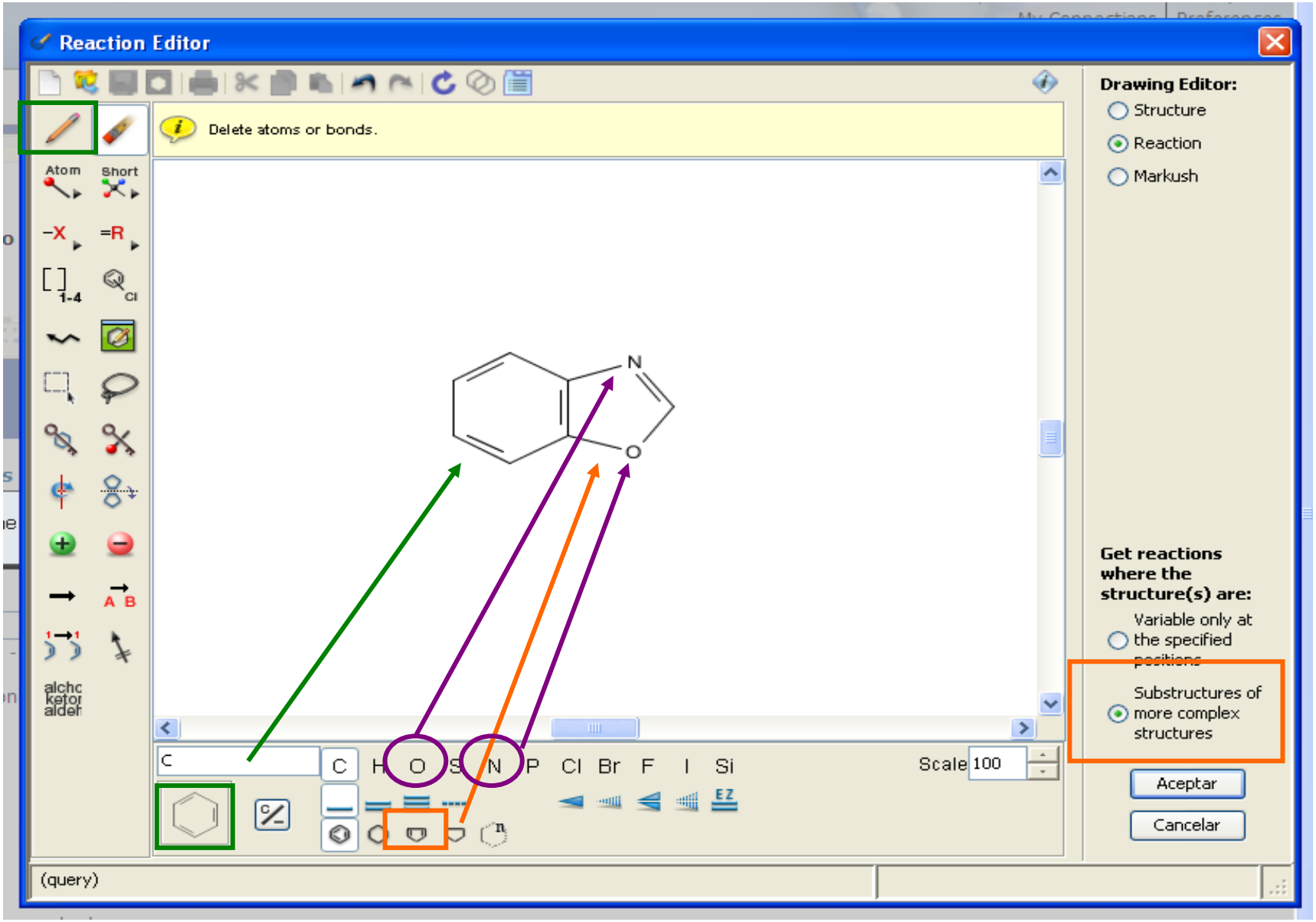
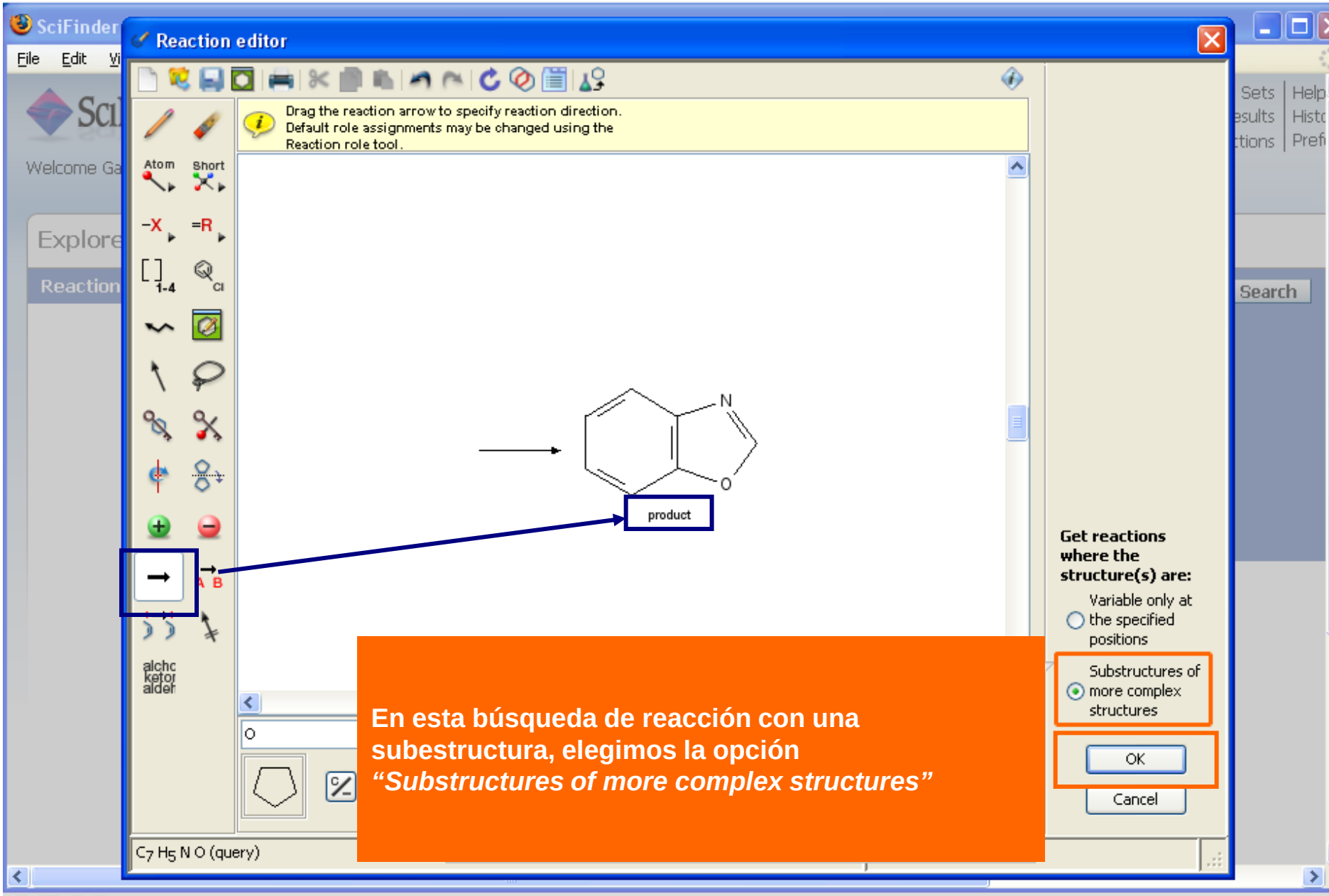
Keep Me Posted Results
Help
History
Welcome Esther Escriche | Sign Out
Explore Reactions
Reaction Structure
Reaction Structure
Click to
Solvent(s)
Select Solvents
Non-participating Functional Group(s)
Select Gro
Number of Steps
Examples: 1, 1 - 3, 1 -,
Classification(s)
Biotransformation
Catalyzed
Chemoselective
Combinatorial
Source(s)
Any source
Patents only
Sources other than patents
Reaction Editor
Delete atoms or bonds.
Atom
Short
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
Aceptar
Cancelar
C H O S N P Cl Br F I Si
Scale 100
(query)


Reaction Editor
Delete atoms or bonds.
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
Aceptar
Cancelar
Scale 100
(query)



En esta búsqueda de reacción con una subestructura, elegimos la opción *"Substructures of more complex structures"*

File Edit View History Bookmarks Tools Help

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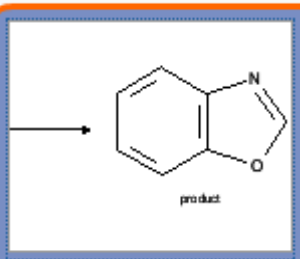
Explore Reactions

Reaction Structure

Reaction Structure



Click image to change structure or view detail

Search type: Allow variability only as specified
Substructure

Search

Una vez dibujada la reacción y dar OK, volvemos a la pantalla de *Explore Reactions*

Solvents — Select Solvents NEW

Number of Steps

Examples: *1, 1 - 3, 1 -, - 3*

Classification(s)

- Biotransformation
- Catalyzed
- Chemoselective
- Electrochemical
- Gas-phase
- Non-catalyzed
- Radiochemical
- Regioselective
- Stereoselective

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Create Keep Me Posted | Reaction Structure substructure > reactions (32564)

Reactions

Se recuperan 32564 reacciones

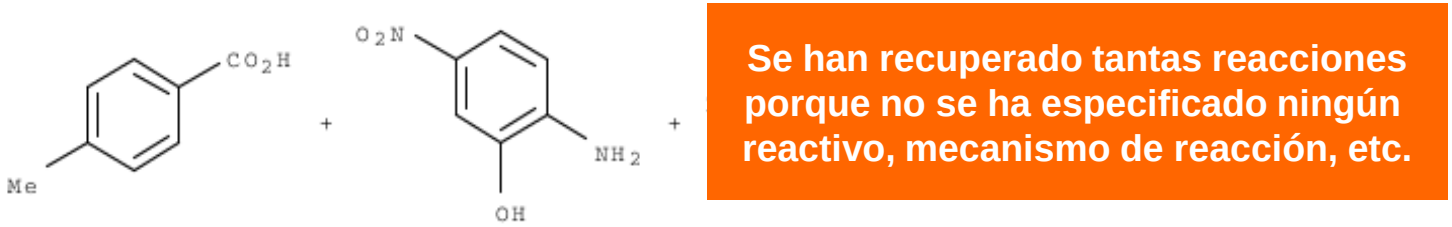
32564 Reactions

Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [15] | 1 2 3 4 5 6 ... 2171

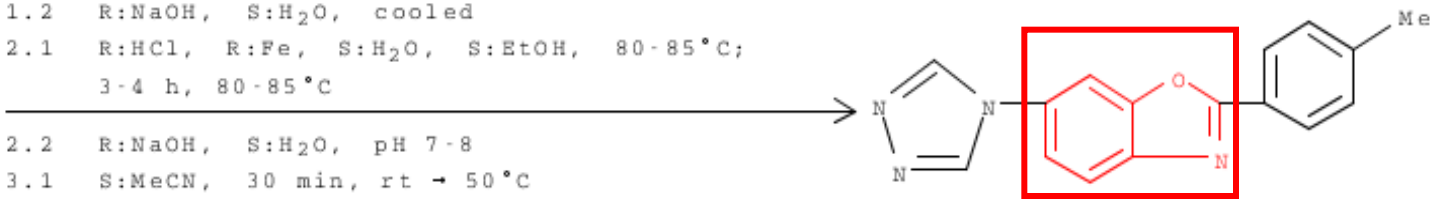
Display:

1. Reaction Detail | Link



Se han recuperado tantas reacciones porque no se ha especificado ningún reactivo, mecanismo de reacción, etc.

1.1 8 h, heated
1.2 R:NaOH, S:H_2O, cooled
2.1 R:HCl, R:Fe, S:H_2O, S:EtOH, 80-85°C; 3-4 h, 80-85°C



2.2 R:NaOH, S:H_2O, pH 7-8
3.1 S:MeCN, 30 min, rt → 50°C
3.2 C:AcOH, S:MeCN, 3 h, 50°C → 120°C; cooled

NOTE: 1) polyphosphoric acid used as reagent in stage 1, excess of NaOH used in stage 2,
Reactants: 4, Reagents: 3, Catalysts: 1, Solvents: 3,
Steps: 3, Stages: 6, Most stages in any one step: 2

Analysis

Sample Analysis

Catalyst

Pd
4-PyNMe2
Pd(PPh3)4
AcOH
Ph2-pentadienone Pd
DMF
Ni
Pd(OH)2
95464-05-4
p-MeC6H4SO3H

Explore References | Explore Substances | Explore Reactions

Saved Answer Sets | Help
Keep Me Posted Results | History
NEW My Connections | Preferences

Gayle Bussell | Sign Out

Reaction Structure substructure > reactions (32564)

Get References

actions 0 Selected | Keep Selected | Remove Selected

Deselect All | Sort by: Accession Number

Para acotar la búsqueda tenemos dos herramientas: Analysis y Refine

Analysis | Refine

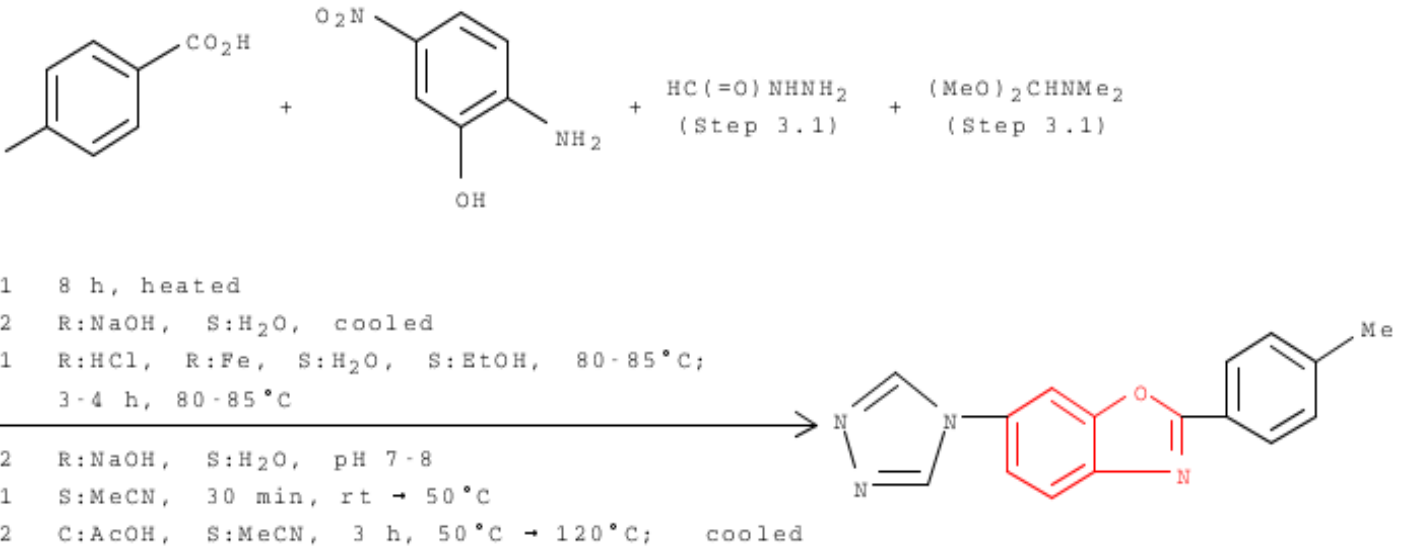
Sample Analysis

Catalyst

- Pd
- 4-PyNMe2
- Pd(PPh3)4
- AcOH
- Ph2-pentadienone Pd
- DMF
- Ni
- Pd(OH)2
- 95464-05-4
- p-MeC6H4SO3H

Display:

Reaction Detail | Link



1 8 h, heated
2 R:NaOH, S:H2O, cooled
1 R:HCl, R:Fe, S:H2O, S:EtOH, 80-85°C;
3-4 h, 80-85°C

2 R:NaOH, S:H2O, pH 7-8
1 S:MeCN, 30 min, rt → 50°C
2 C:AcOH, S:MeCN, 3 h, 50°C → 120°C; cooled

TE: 1) polyphosphoric acid used as reagent in stage 1, excess of NaOH used in stage 2,
Reactants: 4, Reagents: 3, Catalysts: 1, Solvents: 3,

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Explore References | Explore Substances | Explore Reactions

Saved Answer Sets | Help
Keep Me Posted Results | History
My Connections | Preference

Welcome Esther Escriche | Sign Out

Create Keep Me Posted | Reaction Structure substructure > **reactions (54)**

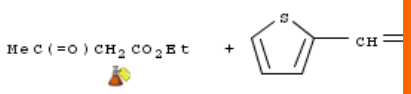
Reactions | Get References | Find Additio Reactions

54 Reactions | 0 Selected | Keep Selected | Remove Se | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [15] | 1 2 3 4

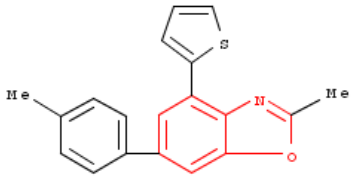
Display:

1. Reaction Detail | Link



De todas las posibilidades que Ofrece esta opción, elegiremos *"Reaction Structure"*.

1.1 R:NaOEt, S:Et_2O, 20 h, rt
1.2 R:AcOH, rt
1.3 R:NaOH, S:H_2O, 6 h, reflux
2.1 R:AcONa, R:H_2NOH·HCl, S:H_2O, S:EtOH, 1 h, reflux
3.1 R:C_5H_5N, S:C_5H_5N, 0-2°C; 2 h, 0°C
4.1 R:NaOEt, S:EtOH, 8 h, reflux



4.2 R:AcOH, acidify
4.3 R:HCl, S:H_2O
4.4 R:AcONa, S:H_2O, 30 min, 70°C
5.1 R:$POCl_3$, S:$POCl_3$, 3 h, reflux
5.2 R:H_2O
6.1 R:DDQ, S:Dioxane, 8 h, 105°C

NOTE: 2) stereoselective, 4) stereoselective, in-situ generated reagent(1st stage), 5) chemoselective,
Reactants: 4, Reagents: 10, Solvents: 6,
Steps: 6, Stages: 12, Most stages in any one step: 4

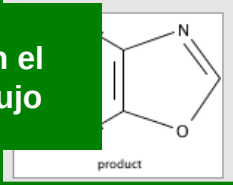
A novel synthetic route for the synthesis of 4,6-diaryl-2-methyl-1,3-benzoxazoles
By Sridharan, V. et al
From Journal of Heterocyclic Chemistry, 42(7), 1321-1330; 2005

Analysis | Refine

Refine by:

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

Reaction Structure:

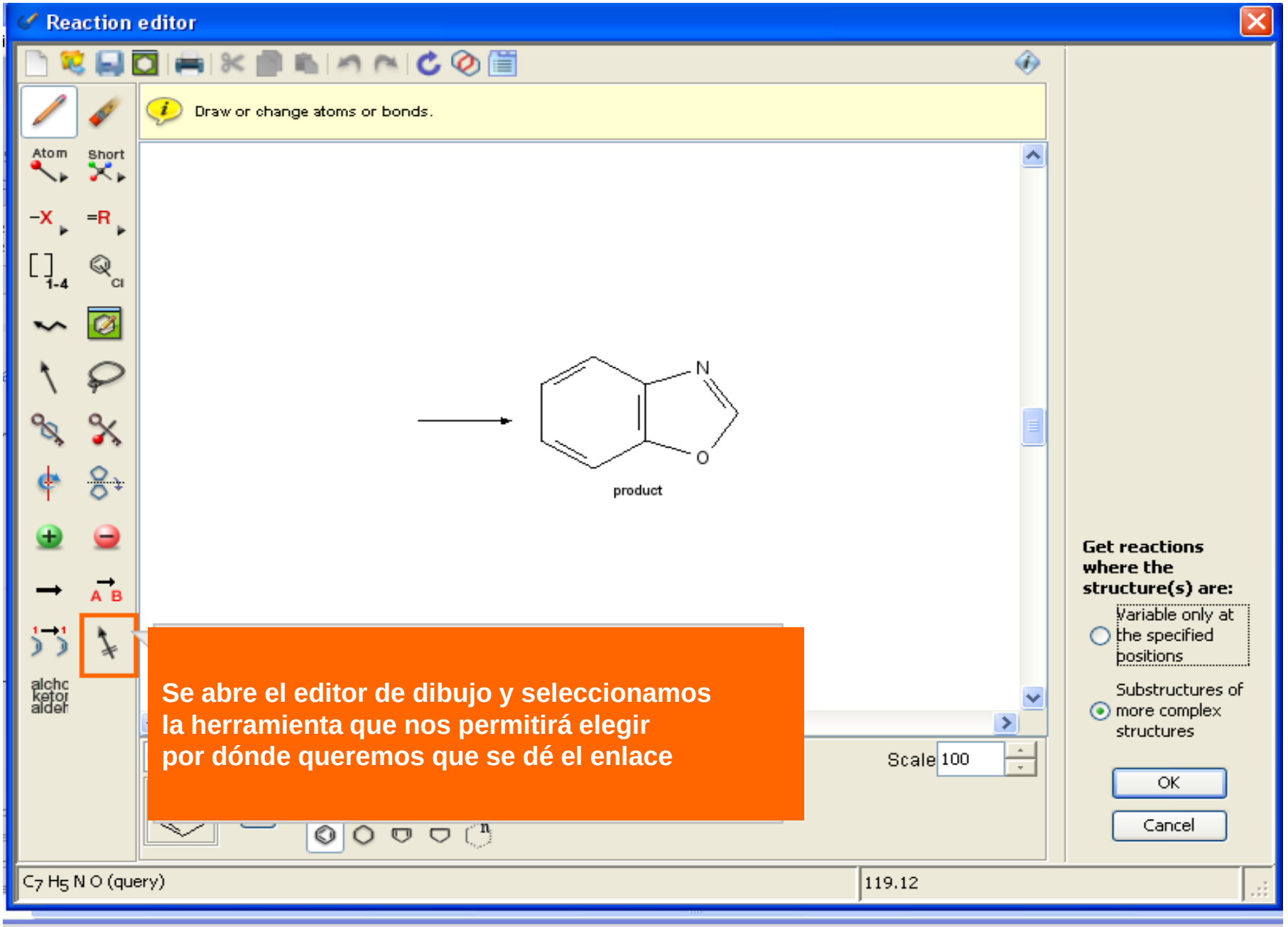


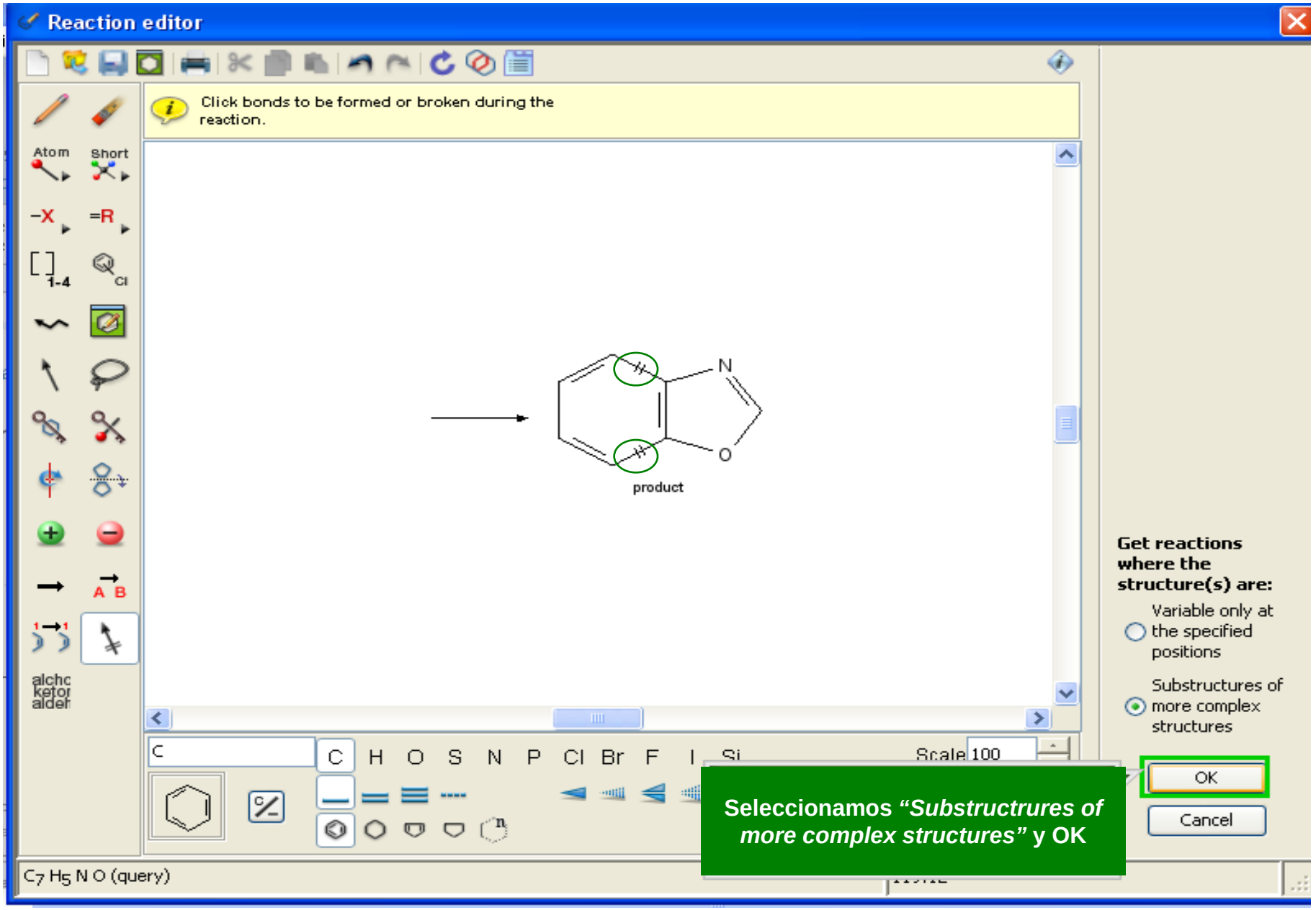
Click image to change structure or view detail

Search type: **Substructure**

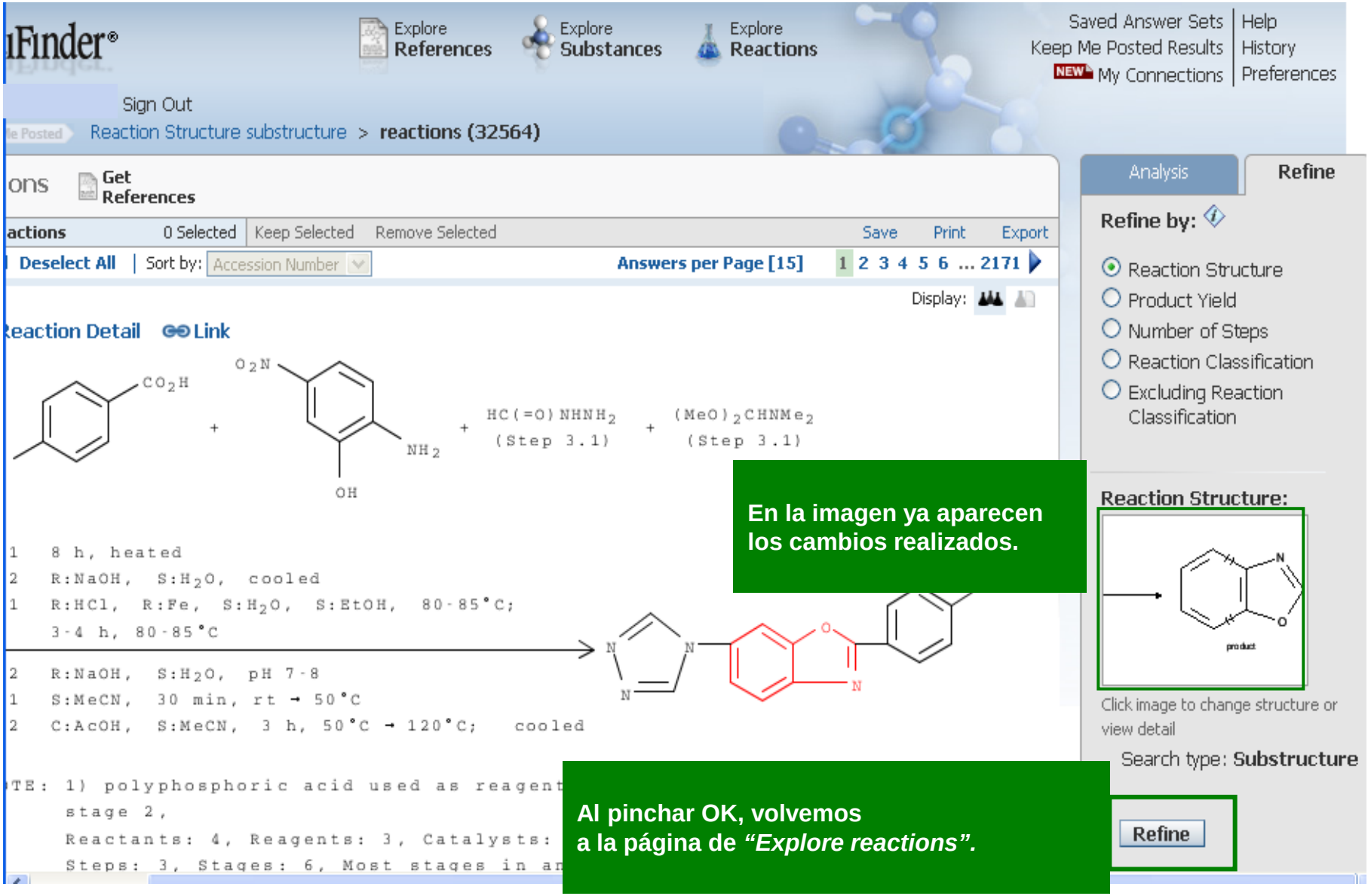
Refine

Pinchamos en el editor de dibujo


Reaction editor
Draw or change atoms or bonds.
Atom
Short
product
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
Scale 100
OK
Cancel
C7 H5 N O (query)
119.12
Se abre el editor de dibujo y seleccionamos la herramienta que nos permitirá elegir por dónde queremos que se dé el enlace



Seleccionamos *"Substructrures of more complex structures"* y OK



En la imagen ya aparecen los cambios realizados.

Al pinchar OK, volvemos a la página de *"Explore reactions".*

SciFinder®

Explore References | Explore Substances | Explore Reactions

Saved Answer Sets | Keep Me Posted Results | NEW My Connections

| Sign Out

Create Keep Me Posted | Reaction Structure substructure > reactions (32564) > refine "substructure" (54)

Reactions

Se recuperan 54 reacciones

54 Reactions

Save | Print | Export

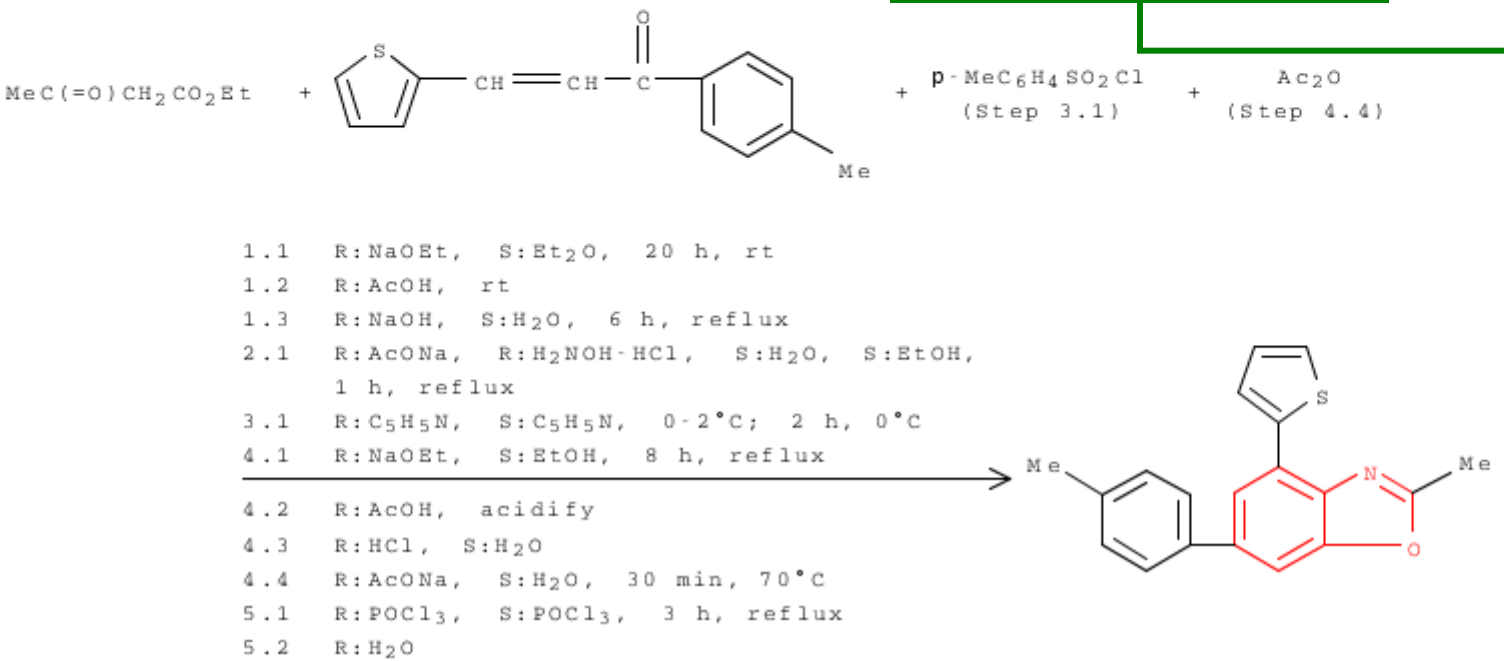
Select All | Deselect All | Sort by: Accession Number

Answers per Page [15] 1 2 3 4

Display:

Pinchamos en el icono de *"one reaction per reference"*

1. Reaction Detail | Link



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Saved Answer Sets | Help
Keep Me Posted Results | Histo
NEW My Connections | Prefi

| Sign Out

Create Keep Me Posted | Reaction Structure substructure > reactions (32564) > **refine "substructure" (54)**

Reactions | Get References

54 Reactions 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All Deselect All | Sort by: Accession Number | Answers per Page [15]

Display: (9 References)

Analysis

Analyze by:

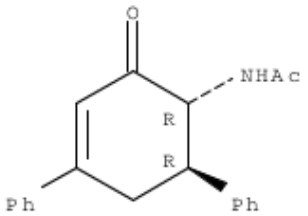
Catalyst

Click bar to view onl within the current a

HCl

Show More

40. 40 Hit Reactions in this Reference



1.1 R
1.2 R
2.1 R.DBU, S.Dioxane, Ph

Relative stereochemistry.

NOTE: 1) chemoselective,
Reactants: 1, Reagents: 3, Solvents: 2,
Steps: 2, Stages: 3, Most stages in any one step: 2

Entre paréntesis aparecen las referencias asociadas a las reacciones.
En este caso, las 54 reacciones están incluidas en 9 referencias.

A novel synthetic route for the synthesis of 4,6-diaryl-2-methyl-1,3-benzoxazoles
By Sridharan, V. et al
From Journal of Heterocyclic Chemistry, 42(7), 1321-1330; 2005

43. 3 Hit Reactions in this Reference

References | Reactions | Answer Sets

54 Reactions | 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [15]

Display: (9 Reactions)

Analyze by: Catalyst

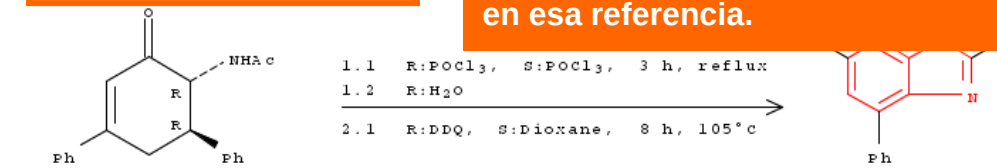
Click bar to view only those reactions within the current answer set

HCl 1

Show More

De esta forma se muestran las reacciones asociadas a cada referencia. Así como el resto de reacciones incluidas en esa referencia.

40. **40 Hit Reactions in this Reference**



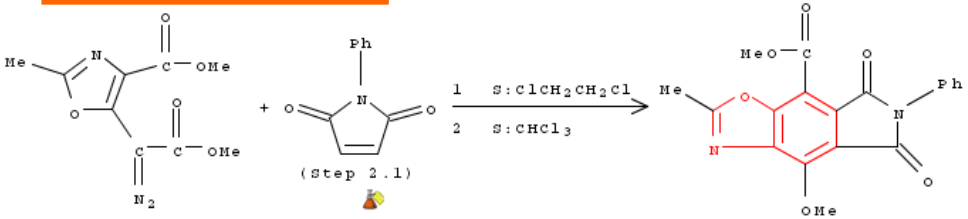
Relative stereochemistry.

Referencia con 40 reacciones (1,2,…,40)

NOTE: 1) chemoselective,
Reactants: 1, Reagents: 3, Solvents: 2,
Steps: 2, Stages: 3, Most stages in any one step: 2

A novel synthetic route for the synthesis of 4,6-diaryl-2-methyl-1,3-benzoxazoles
By Sridharan, V. et al
From Journal of Heterocyclic Chemistry, 42(7), 1321-1330; 2005

43. **3 Hit Reactions in this Reference**



Referencia con 3 reacciones (41, 42, 43)

NOTE: 1) 30 MIN, DIRHODIUM TETRAACETATE, 2) 2 H,
Reactants: 2, Solvents: 2,
Steps: 2, Stages: 2

Synthesis and reactions of a novel furo[3,4-d]oxazole
By Reck, Stephan and Friedrichsen, Willy
From Journal of Organic Chemistry, 63(22), 7680-7686; 1998

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Explore References | Explore Substances | Explore Reactions

Saved Answer Sets | Help
Keep Me Posted Results | History
My Connections | Preferences

Welcome Esther Escriche | Sign Out

Create Keep Me Posted | Reaction Structure substructure > **reactions (54)** > reactions in **"New Perspectives in Oxazole Ch..." (2)**

Reactions | Get References | Find Additional Reactions | Combine Answer Sets

54 Reactions | 40 Selected | Keep Selected | Remove Selected | Print | Export

Select All | Deselect All | Sort by: Accession Number | wers per Page [15]

(9 Reactions)

Analysis | Refine

Analyze by:

Catalyst

Click bar to view only those reactions within the current answer set

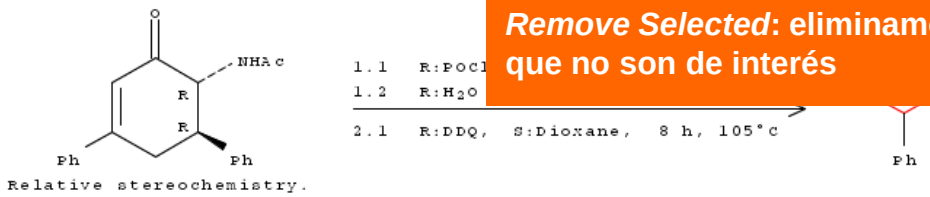
HCl 1

Show More

***Keep Selected*: seleccionamos las reacciones que nos interesan.**

***Remove Selected*: eliminamos las reacciones que no son de interés**

40. **40 Hit Reactions in this Reference**

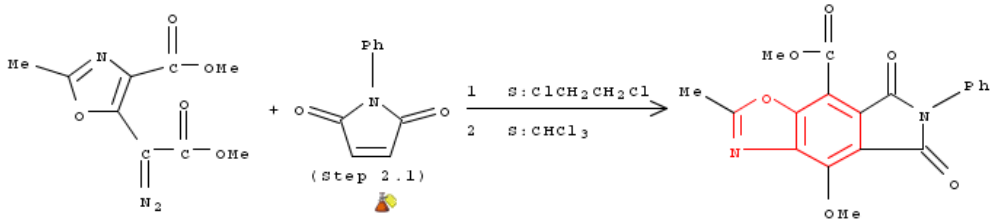


Relative stereochemistry.

NOTE: 1) chemoselective,
Reactants: 1, Reagents: 3, Solvents: 2,
Steps: 2, Stages: 3, Most stages in any one step: 2

A novel synthetic route for the synthesis of 4,6-diaryl-2-methyl-1,3-benzoxazoles
By Sridharan, V. et al
From Journal of Heterocyclic Chemistry, 42(7), 1321-1330; 2005

43. **3 Hit Reactions in this Reference**



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HCl 1

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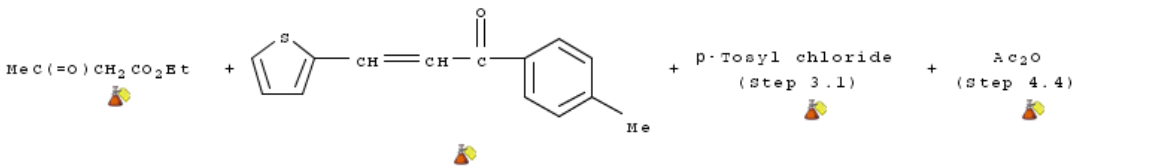
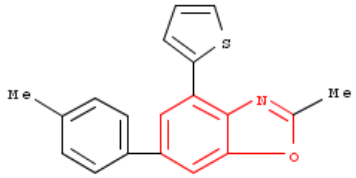
1. **Reaction Detail** Link



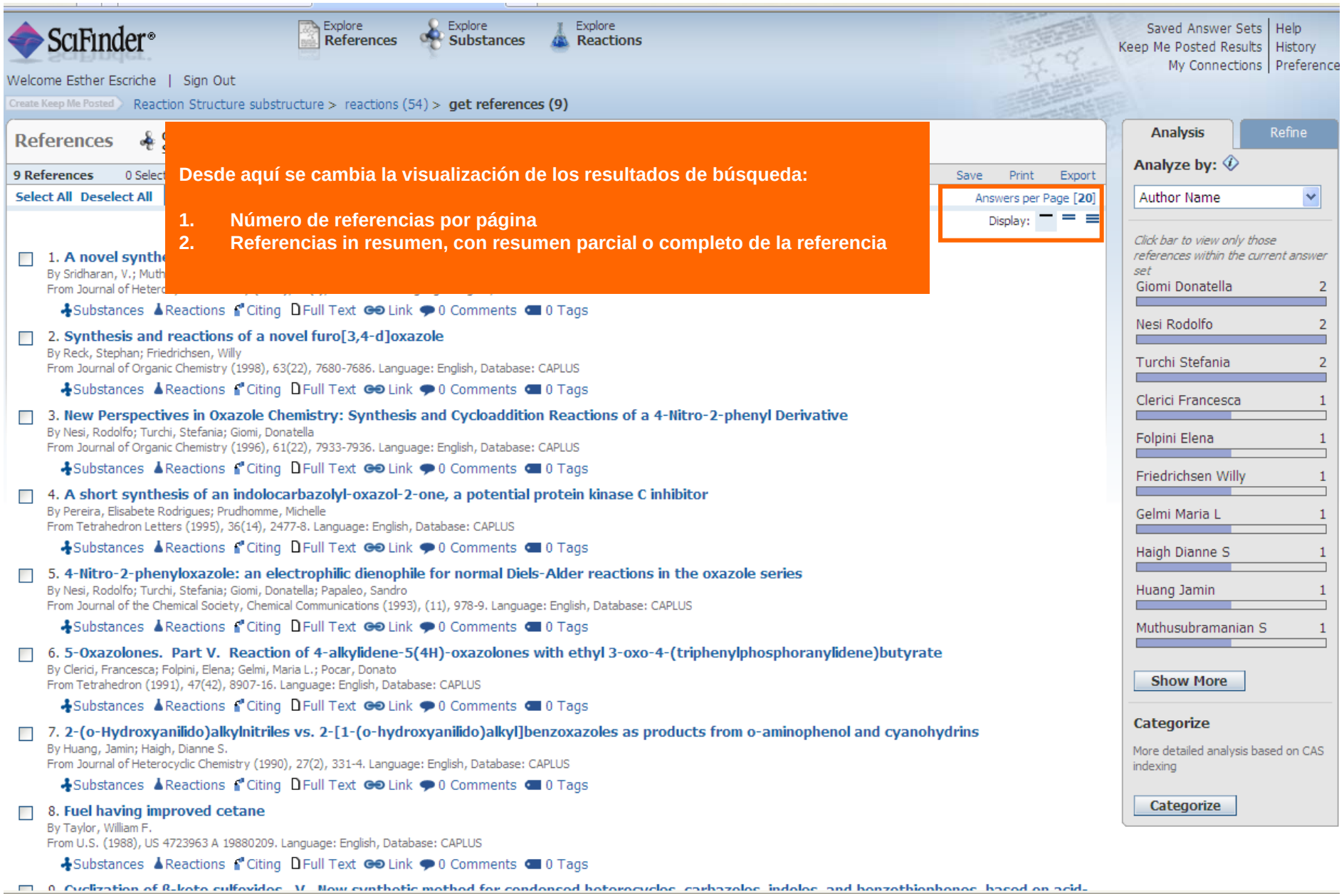
1.1 R:NaOEt, S:Et_2O, 20 h, rt
1.2 R:AcOH, rt
1.3 R:NaOH, S:H_2O, 6 h, reflux
2.1 R:AcONa, R:$H_2NOH \cdot HCl$, S:H_2O, S:EtOH, 1 h, reflux
3.1 R:C_5H_5N, S:C_5H_5N, 0-2°C; 2 h, 0°C
4.1 R:NaOEt, S:EtOH, 8 h, reflux



4.2 R:AcOH, acidify
4.3 R:HCl, S:H_2O
4.4 R:AcONa, S:H_2O, 30 min, 70°C
5.1 R:$POCl_3$, S:$POCl_3$, 3 h, reflux
5.2 R:H_2O
6.1 R:DDQ, S:Dioxane, 8 h, 105°C

NOTE: 2) stereoselective, 4) stereoselective, in-situ generated reagent(1st stage), 5) chemoselective,
Reactants: 4, Reagents: 10, Solvents: 6,
Steps: 6, Stages: 12, Most stages in any one step: 4

A novel synthetic route for the synthesis of 4,6-diaryl-2-methyl-1,3-benzoxazoles
By Sridharan, V. et al
From Journal of Heterocyclic Chemistry, 42(7), 1321-1330; 2005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Reaction Structure substructure > reactions (54) > get references (9)
References
9 References
Select All Deselect All
Save Print Export
Answers per Page [20]
Display:
Desde aquí se cambia la visualización de los resultados de búsqueda:
1. Número de referencias por página
2. Referencias in resumen, con resumen parcial o completo de la referencia
1. A novel synthe
By Sridharan, V.; Muth
From Journal of Hetero
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
2. Synthesis and reactions of a novel furo[3,4-d]oxazole
By Reck, Stephan; Friedrichsen, Willy
From Journal of Organic Chemistry (1998), 63(22), 7680-7686. Language: English, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
3. New Perspectives in Oxazole Chemistry: Synthesis and Cycloaddition Reactions of a 4-Nitro-2-phenyl Derivative
By Nesi, Rodolfo; Turchi, Stefania; Giomi, Donatella
From Journal of Organic Chemistry (1996), 61(22), 7933-7936. Language: English, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
4. A short synthesis of an indolocarbazolyl-oxazol-2-one, a potential protein kinase C inhibitor
By Pereira, Elisabete Rodrigues; Prudhomme, Michelle
From Tetrahedron Letters (1995), 36(14), 2477-8. Language: English, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
5. 4-Nitro-2-phenyloxazole: an electrophilic dienophile for normal Diels-Alder reactions in the oxazole series
By Nesi, Rodolfo; Turchi, Stefania; Giomi, Donatella; Papaleo, Sandro
From Journal of the Chemical Society, Chemical Communications (1993), (11), 978-9. Language: English, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
6. 5-Oxazolones. Part V. Reaction of 4-alkylidene-5(4H)-oxazolones with ethyl 3-oxo-4-(triphenylphosphoranylidene)butyrate
By Clerici, Francesca; Folpini, Elena; Gelmi, Maria L.; Pocar, Donato
From Tetrahedron (1991), 47(42), 8907-16. Language: English, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
7. 2-(o-Hydroxyanilido)alkylnitriles vs. 2-[1-(o-hydroxyanilido)alkyl]benzoxazoles as products from o-aminophenol and cyanohydrins
By Huang, Jamin; Haigh, Dianne S.
From Journal of Heterocyclic Chemistry (1990), 27(2), 331-4. Language: English, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
8. Fuel having improved cetane
By Taylor, William F.
From U.S. (1988), US 4723963 A 19880209. Language: English, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
Analysis
Refine
Analyze by:
Author Name
Click bar to view only those references within the current answer set
Giomi Donatella 2
Nesi Rodolfo 2
Turchi Stefania 2
Clerici Francesca 1
Folpini Elena 1
Friedrichsen Willy 1
Gelmi Maria L 1
Haigh Dianne S 1
Huang Jamin 1
Muthusubramanian S 1
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En esta sesión formativa hemos realizado:

1. **Una búsqueda por *"explore reactions"* empleando como producto una subestructura.**
2. **Especificación de los enlaces para que se dé la reacción**
3. **Cambio de la visualización para ver las referencias asociadas a las reacciones que se han recuperado.**
1. **Mantener o eliminar reacciones de interés o no.**
2. **Recuperar las referencias asociadas a las reacciones.**
3. **Cambiar la visualización de estas referencias.**