Answer for a request from chemists: How to use IJC as a lab notebook?

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ChemAxon

ChemAxon User Meeting, Budapest, March 20-22, 2018

HAS-RCNS Medicinal Chemistry Research Group

- **Group leader**: György Miklós Keserű DSc, FRSC
- **Lab staff**:
  – Senior research staff: 8
  – Junior research staff: 10
  – Undergraduates: 19
  – Technical assistance: 1

- **Publications** 2013-2017: 85 medchem/orgchem papers with 676 independent citations (799 all)
- We have international visibility indicated by **13 papers in top 5% cited**

HAS-RCNS Medicinal Chemistry Research Group

- **Research fields:**
  - GPCRs, particularly dopamine D2/D3, cannabinoid CB1, mGluR5, 5HT6,7,2B, Beta1,2
  - Oncology: JAK, STAT, Ras, pediatric oncology
  - Immunoproteasome
  - Covalent fragment design
  - Antibody labelling
  - Intrinsically disordered proteins

- **Collaborations:**

Collaborators	Domestic	International
Industry	Gedeon Richter EGIS TEVA KCH Mcule, Femtonics, KinetoLab	GSK AstraZeneca Novartis Astex, Heptares, Vernalis BioBlocks
Academia	István Katona, Balázs Györffy, Perczel András, BeátaVértessy, Martinek Tamás, Tímár József, Tóth Gergely, Buday László, Mándity István, Balázs Jójárt, Árpád Márki	Holger Stark, Peter Tompa, Vijay Chudasama, Rob Leurs, Chris de Graaf, Peter Sayeski, Aurun Shukla, Stanislav Gobec, Andrzej Bojarski, Xavier Barril, Sandor Vajda, Richard Moriggl, Peter Kolb, Gillian Baker

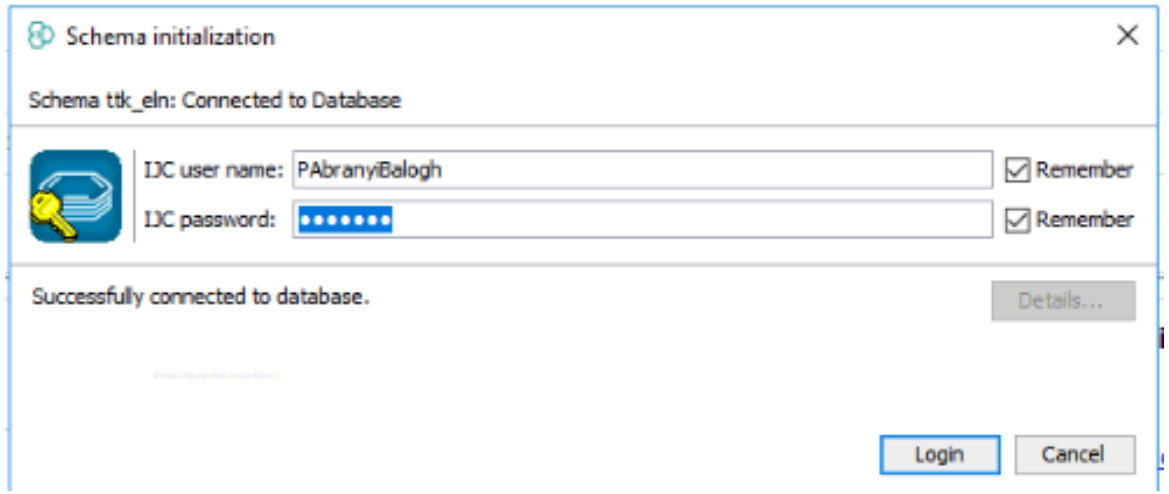
We built up a global collaboration network with partners in the EU, US, and Asia

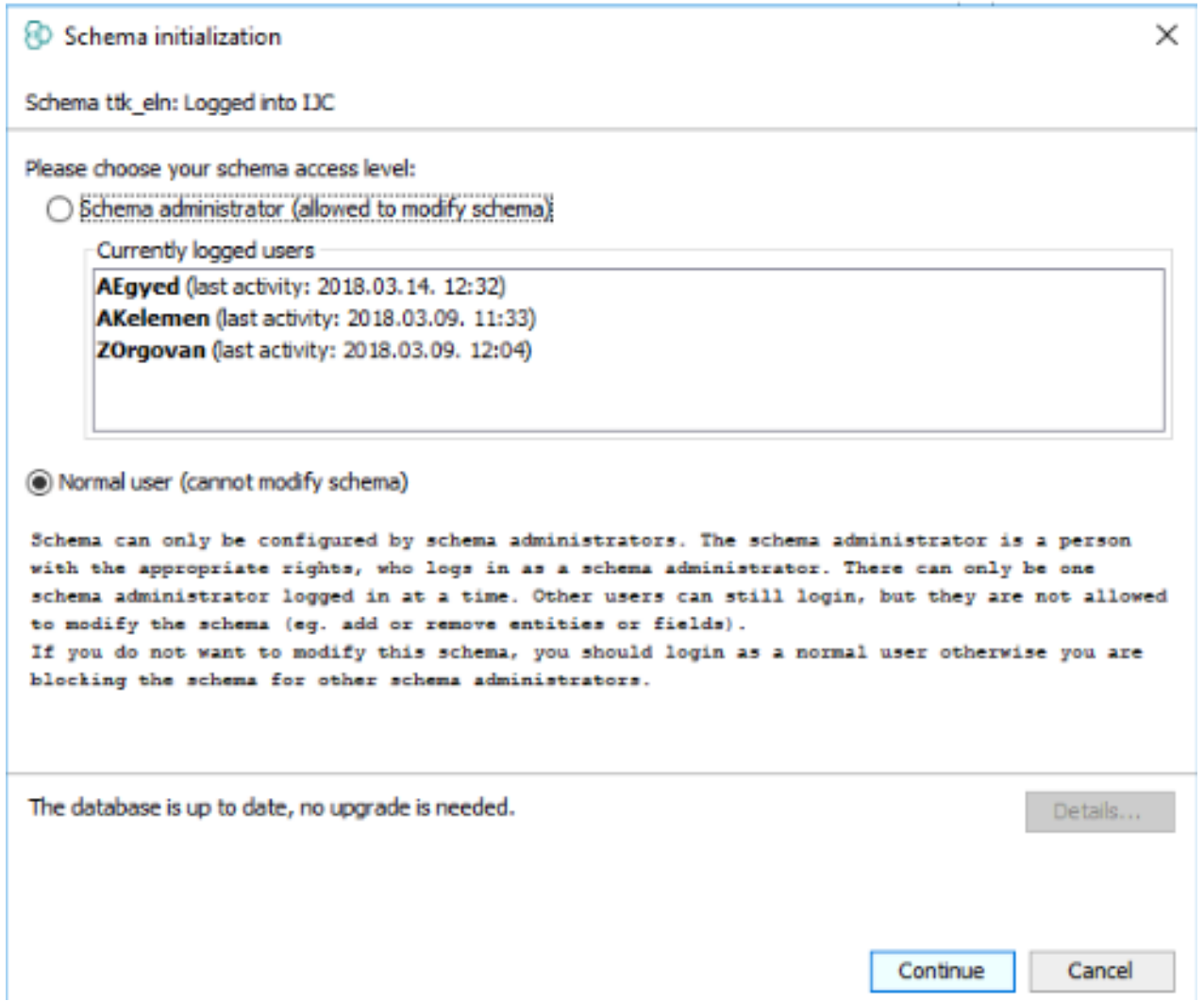
Questions to be answered

- More than 30 people working in the lab, the synthetic information in one year can be more than 5000 reactions.
- This huge chemical experience and knowledge is on paper. How to search? How to share effectively?
- The reactant database should be up-to-date, but for 5700 compounds the manual registry of the consumption is complicated.
- The ELN systems available commercially are much too expensive for an academic research group in Hungary, but for most of the competitors it makes the synthetic work more effective.

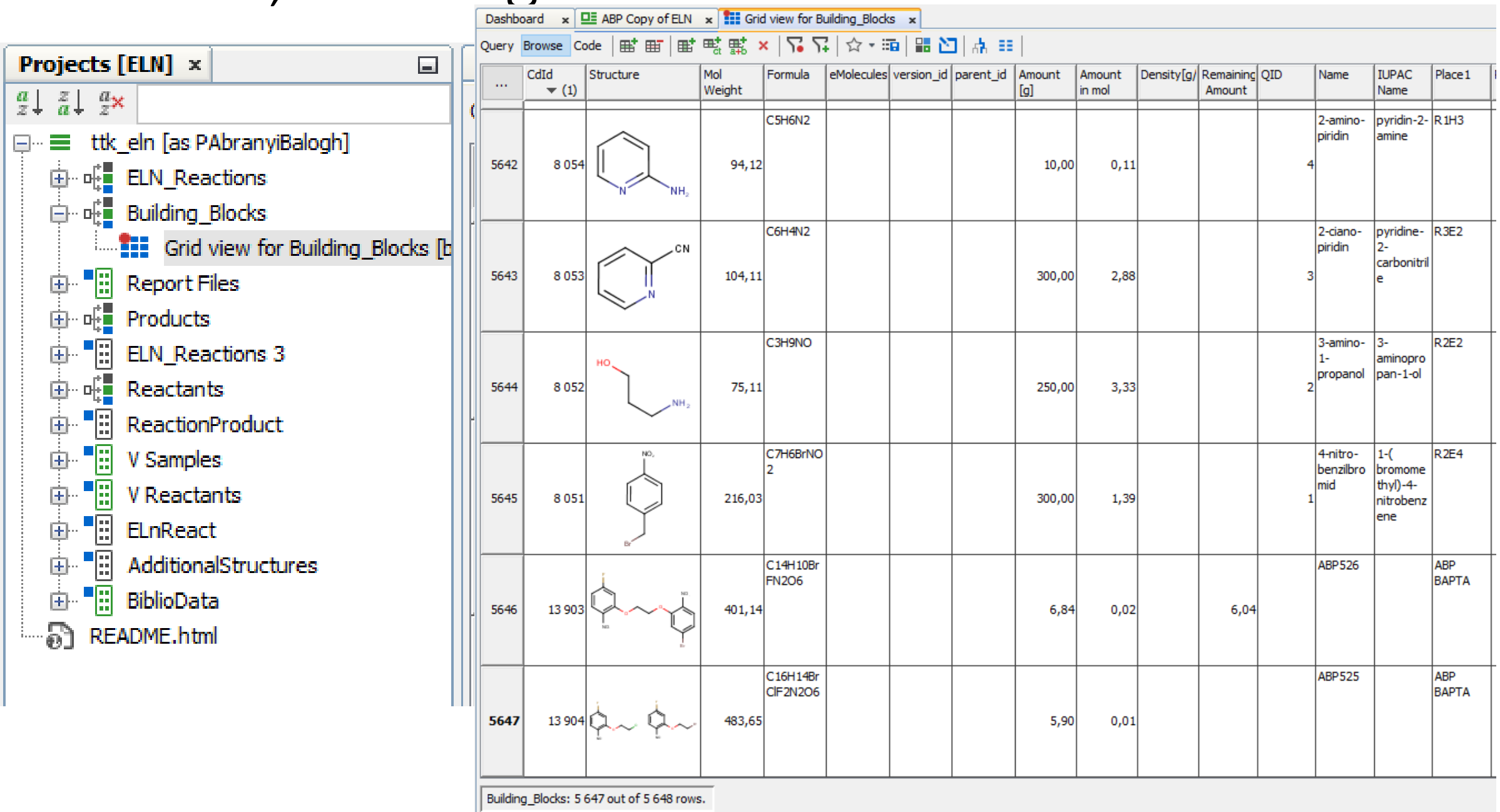
The answer from ChemAxon: An IJC project used as a basic ELN

User management



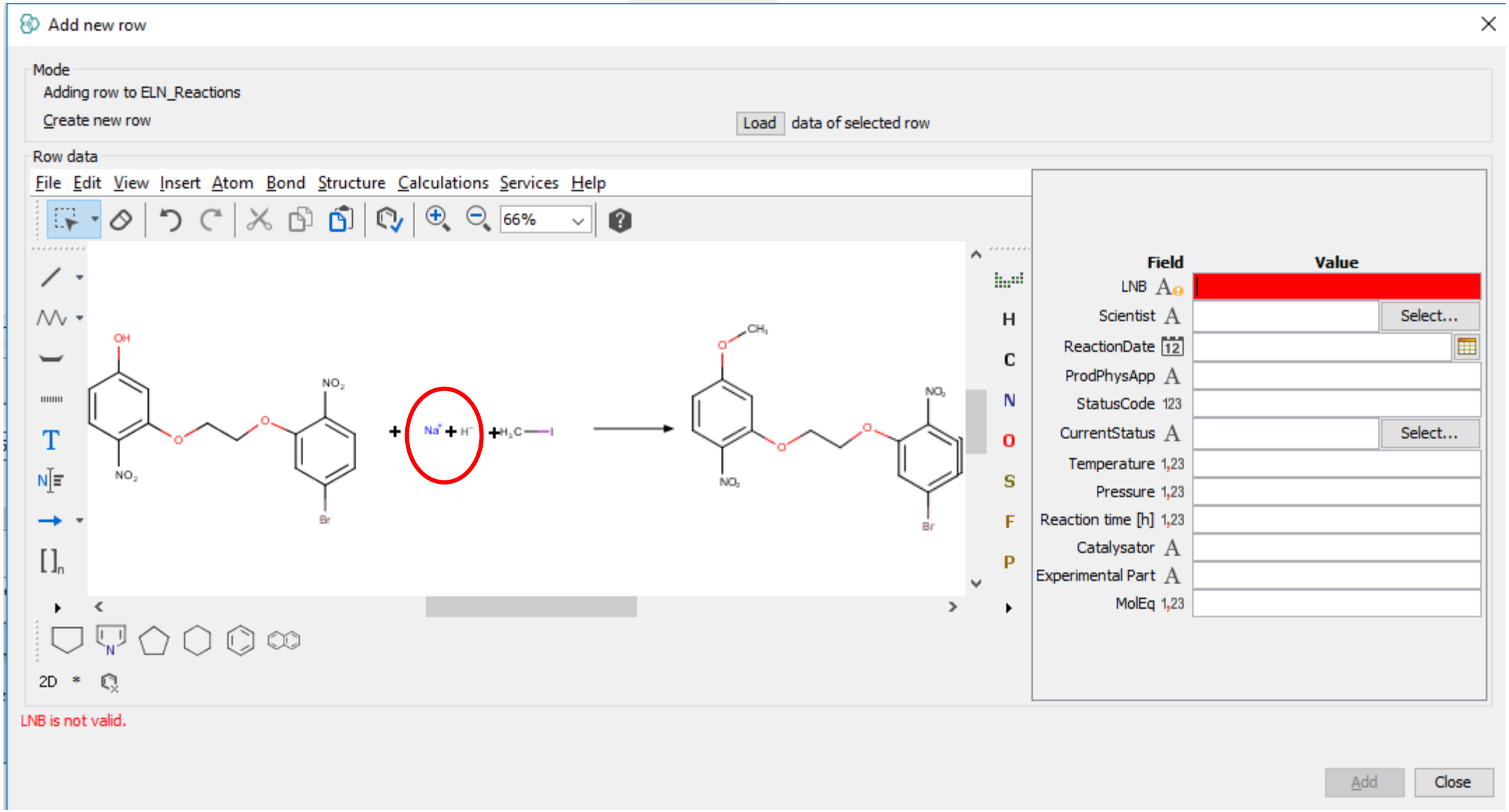


Reactant, building block database



...	CdId (1)	Structure	Mol Weight	Formula	eMolecules	version_id	parent_id	Amount [g]	Amount in mol	Density[g/	Remaining Amount	QID	Name	IUPAC Name	Place1
5642	8 054		94,12	C5H6N2				10,00	0,11			4	2-amino-piridin	pyridin-2-amine	R1H3
5643	8 053		104,11	C6H4N2				300,00	2,88			3	2-ciano-piridin	pyridine-2-carbonitrile	R3E2
5644	8 052		75,11	C3H9NO				250,00	3,33			2	3-amino-1-propanol	3-aminopropan-1-ol	R2E2
5645	8 051		216,03	C7H6BrNO2				300,00	1,39			1	4-nitro-benzilbromid	1-(bromomethyl)-4-nitrobenzene	R2E4
5646	13 903		401,14	C14H10BrFN2O6				6,84	0,02		6,04		ABP526		ABP BAPTA
5647	13 904		483,65	C16H14BrClF2N2O6				5,90	0,01				ABP525		ABP BAPTA

Reaction handling



Add new row

Mode

Adding row to ELN_Reactions

Create new row

Load data of selected row

Row data

File Edit View Insert Atom Bond Structure Calculations Services Help

66%

Field	Value
LNB	
Scientist	Select...
ReactionDate	
ProdPhysApp	
StatusCode	
CurrentStatus	Select...
Temperature	
Pressure	
Reaction time [h]	
Catalysator	
Experimental Part	
MolEq	

LNB is not valid.

Add Close

Cut Ctrl+X
Copy Ctrl+C
Copy As... Ctrl+K
Delete
Group... Ctrl+G
Add
No Structure
Edit Properties...
Check Structure Ctrl+R
Merge Reactants
Transformation
Align
Distribute
Align and Distribute
Format...
Add to My Templates

tants: 2/159. Building_Blocks: 1/5 648. V Samples: 1/88. V React

eact: 0/71. AdditionalStructures: 1/46. Products: 0/4. Project: 1/29. BiblioData: 0/5.

Add new row

Mode

Adding row to ELN_Reactions

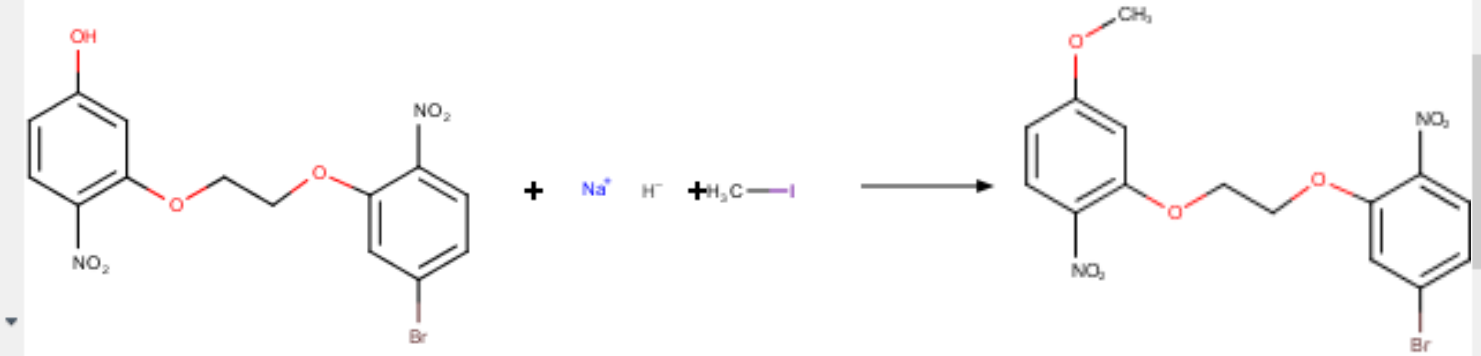
Create new row

Load data of selected row

Row data

File Edit View Insert Atom Bond Structure Calculations Services Help

66%



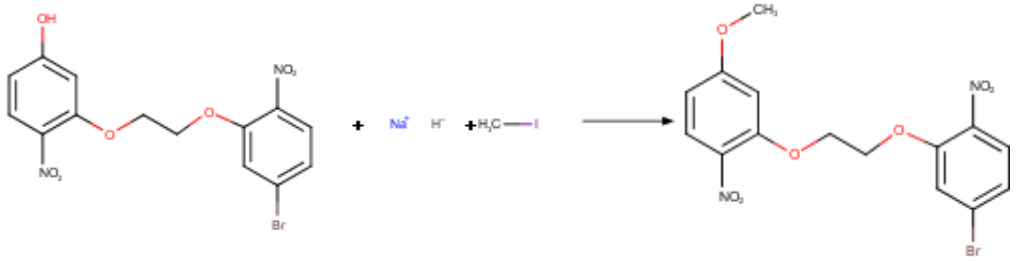
Field	Value
LNB	ABP554
Scientist	Ábrányi-Balogh Péter (Select...)
ReactionDate	
ProdPhysApp	
StatusCode	
CurrentStatus	(Select...)
Temperature	25
Pressure	
Reaction time [h]	2
Catalysator	
Experimental Part	
MolEq	2

Add Close

Dashboard | ABP Copy of ELN

Design | Query | Browse | Code

Reaction structure



Analyse Reaction | Refresh Products | Clear Reactants | Clear Products

Experimental part (new line Ctrl+Enter)

LNB: ABP554

ReactionDate:

Scientist: Ábrányi-Balogh Péter

CurrentStatus:

MolEq: 2,00

Reaction time [h]: 2,00

T [°C]: 25,00

P[bar]:

Catalysator:

AddSketch | Reports

Additional Drawings

Structure

Reactants

...	#React	ReactantC	Mw	Density	Amount [mmol]	Stochion	Volume Needed [mL]	Amount Needed [g]	Amount Consumed	Last

Building_Blocks

...	Structure	Mol Weigh	Remaining Amount	QID	Name	IUPA Nam	Place	Place	Place	Place 4	Place 5	LNB_R	Produc	User	CAS

ReactionProduct

...	Structure	Mol Weight	Formul	LNB_R	Usernan	Eq.Amc [mmol]	Stoichi	Calcula Amour	Measured Amount	Calc. Yield [%]	R_Num	Add2BB

Project

ProjectName

BiblioData

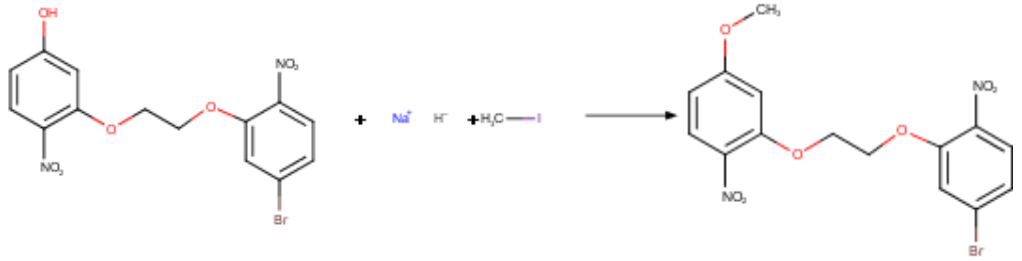
Journal | Yea

ELN_Reactions: 46/46. Report Files: 0/0. Reactants: 0/159. Building_Blocks: 0/5 648. V Samples: 0/88. V Reactants: 0/176. ReactionProduct: 0/94. ELnReact: 0/71. AdditionalStructures: 0/46. Products: 0/4. Project: 0/29. BiblioData: 0/5.

Dashboard | ABP Copy of ELN

Design | Query | Browse | Code

Reaction structure



Analyse Reaction | Refresh Products | Clear Reactants | Clear Products

Experimental part (new line Ctrl+Enter)

Reaction:
Work-up:
Purification:

LNB: **ABP554**

ReactionDate:

Scientist: Ábrányi-Balogh Péter

CurrentStatus:

Reactants

#	#React	ReactantC	Mw	Density	Amount [mmol]	Stochion	Volume Needed [mL]	Amount Needed [g]	Amount Consumed
1	1	13 906	399,15		2,00	1,00		0,798	
2	0	8 191	24,00		2,00	1,00		0,048	
3	0	10 211	24,00		2,00	1,00		0,048	
4	0	10 644	24,00		2,00	1,00		0,048	

MolEq: 2,00

Reaction time [h]: 2,00

T [°C]: 25,00

P[bar]:

Catalysator:

Building_Blocks

#	Structure	Mol Weigh	Remaining Amount	QID	Name	IUPA Nam	Place	Place	Place	Place 4	Place 5	LNB_R	Produc	User	CAS
1	Na⁺ H⁻	24,00		2 814	Sigma 5g, Fluka 500g		R3H 2, Vas0 3/2, Vas0 2								

ReactionProduct

#	Structure	Mol Weight	Formul	LNB_R	Usernan	Eq.Amc [mmol]	Stoichi	Calcula Amour	Measured Amount	Calc. Yield [%]	R_Num	Add2BB
1		399,15	C14H11BrN2O7	ABP554	PAbranyiBalogh	2,00	1,00	0,80			0	

AddSketch | Reports

Additional Drawings

Structure

1

Project

ProjectName

BiblioData

Journal | Yea

ELN_Reactions: 46/46. Report Files: 0/0. Reactants: 10/159. Building_Blocks: 1/5 649. V Samples: 1/88. V Reactants: 1/176. ReactionProduct: 1/95. ELnReact: 0/71. AdditionalStructures: 1/47. Products: 0/4. Project: 0/29. BiblioData: 0/5.

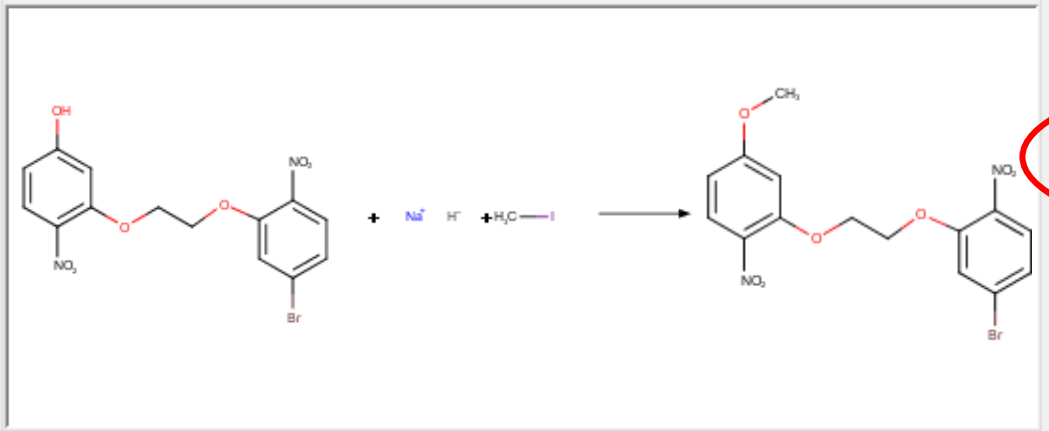
Dashboard | ABP Copy of ELN

Design | Query | Browse | Code

Analyse Reaction | Refresh Products | Clear Reactants | Clear Products

AddSketch | Reports

Reaction structure



Experimental part (new line Ctrl+Enter)

Reaction: NaH is suspended in 10 mL of DMF, and phenol is added dropwise in 10 mL DMF. After 30 min, MeI is added. Stirred for an additional hour.
Work-up: 10 mL of icy water and 10 mL cc Na2CO3 solution is added. Extracted with 3x20 mL EtOAc.
Purification: -

Additional Drawings

Structure

1

LNB: **ABP554**

ReactionDate:

Scientist: Ábrányi-Balogh Péter

CurrentStatus:

MolEq: 2,00

Reaction time [h]: 2,00

T [°C]: 25,00

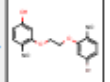
P[bar]:

Catalysator:

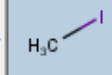
Reactants

	#React	ReactantC	Mw	Density	Amount [mmol]	Stochion	Volume Needed [mL]	Amount Needed [g]	Amount Consumed	Last
1	1	13 906	399,15		2,00	1,00		0,798	0,80	201
2	0	10 211	24,00	0,60	2,00	1,10	0,088	0,053	0,09	201
3	2	10 104	141,94	2,28	2,00	1,10	0,137	0,312	0,14	201

ReactionProduct

	Structure	Mol Weight	Formul	LNB_R	Usernan	Eq.Amo [mmol]	Stoichi	Calcula Amour	Measured Amount	Calc. Yield [%]	R_Num	Add2BB
1		399,15	C14H11BrN2O7	ABP554	PAbranyiBalogh	2,00	1,00	0,80			0	☐

Building_Blocks

	Structure	Mol Weigh	Remaining Amount	QID	Name	IUPA Nam	Place	Place	Place	Place 4	Place 5	LNB_R	Produc	User	CAS
1		141...		2 707	ABCR 50g, Sigma 100 ml		É501/H01/3, É502/H04/1								

Project

ProjectName

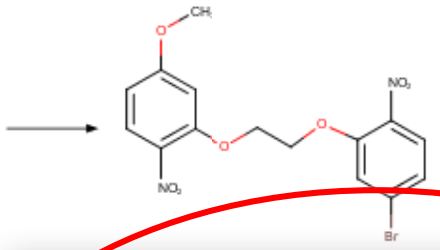
BiblioData

Journal | Year

ELN_Reactions: 46/46. Report Files: 0/0. Reactants: 3/152. Building_Blocks: 1/5 649. V Samples: 1/88. V Reactants: 1/176. ReactionProduct: 1/95. ELnReact: 0/71. AdditionalStructures: 1/47. Products: 0/4. Project: 0/29. BiblioData: 0/5.

Dashboard | ABP Copy of ELN

Design | Query | Browse | Code



Analyse Reaction | Refresh Products | Clear Reactants | Clear Products

Experimental part (new line Ctrl+Enter)

Reaction: NaH is suspended in 10 mL of DMF, and phenol is added dropwise in 10 mL DMF. After 30 min, MeI is added. Stirred for an additional hour.
Work-up: 10 mL of icy water and 10 mL cc Na2CO3 solution is added. Extracted with 3x20 mL EtOAc.
Purification: -

ReactionDate: 2018.03.22. 15:54:30

Scientist: Ábrányi-Balogh Péter

CurrentStatus:

Reaction time [h]: 2,00

T [°C]: 25,00

P[bar]:

Catalysator:

Formul	LNB_R	Usernan	Eq.Amo [mmol]	Stoichi	Calcula Amour	Measured Amount	Calc. Yield [%]	R_Num	Add2BB
C14H11BrN2O7	ABP554	PAbranyiBalogh	2,00	1,00	0,80			0	☐

Edit CurrentStatus value

Type value: Idea

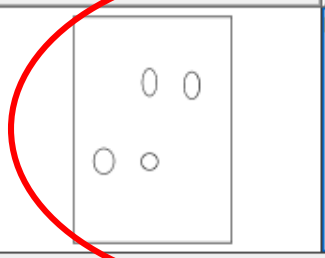
Select from list:
- Idea
- PurchasingReactants
- Reaction
- Purification
- Done
- Unsuccessful
- On-hold

Showing 7 out of 7 values

Save | Clear value | Cancel

AddSketch | Reports

Additional Drawings

...	Structure	Comment
1		DCM:MeOH 19:1

Project

...	ProjectName
1	Femtonics - Bapta

BiblioData

...	Journal	Year	Vol	First Page	Combined	Link
1	JMC	2 001	13	123		http:/

ELN_Reactions: 46/46. Report Files: 0/0. Reactants: 3/152. Building_Blocks: 1/5 649. V Samples: 1/88. V Reactants: 1/176. ReactionProduct: 1/95. ELnReact: 0/71. AdditionalStructures: 1/47. Products: 0/4. Project: 1/30. BiblioData: 1/6.

LNB: **ABP554**

ReactionDate: 2018.03.22. 15:54:30

Scientist: Ábrányi-Balogh Péter

CurrentStatus: Done

MolEq: 2,00

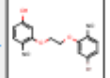
Reaction time [h]: 2,00

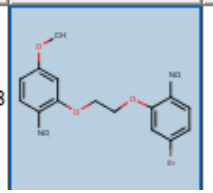
T [°C]: 25,00

P[bar]:

Catalysator:

ReactionProduct

...	Structure	Mol Weight	Formul	LNB_R	Usernan	Eq.Amc [mmol]	Stoichi	Calcula Amou	Measured Amount	Calc. Yield [%]	R_Num	Add2BB
1		399,15	C14H11BrN2O7	ABP554	PAbranyiBalogh	2,00	1,00	0,80	0,70	88	0	☑

...	CdId (1)	Structure	Mol Weight	Formula	eMolecules	version_id	parent_id	Amount [g]	Amount in mol	Density[g/	Remaining Amount	QID	Name	IUPAC Name	Place1	Place2	Place3	Place 4	Place 5	LNB_Ref	Username	ProductID	CAS
1	13 908		413,18	C15H13BrN2O7				0,80	0,00											ABP554	PAbranyiBalogh	743	

stry Tools Window Help

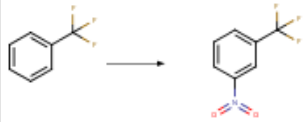
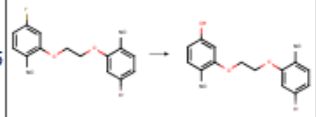
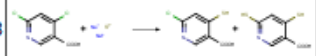
Search (Ctrl+I)

425,8/505,0MB

46 / 46

Dashboard | ABP Copy of ELN | Grid view for ELN_Reactions | Grid view for Building_Blocks

Query Browse Code

...	CdId	Reaction structure	LNB	Scientist	ReactionDate	ProdPhysApp	StatusCode	Temperature	Pressure	Reaction time [h]	Catalysator	Experimental Part
												Work-up:A reakci...
41	104		CsD-273	Csányi Dorottya	2018.01.23. 14:4...			0,00				Reaction: Work-up: Purification:
42	105		ABP551	Ábrányi-Balogh Péter	2018.03.19. 9:48...			25,00				Reaction: 10 mL DMSO-hoz adom a nitrovegyületet, majd 800 uL 20%-os NaOH oldatot csepegtetek hozzá és RT kevertetem...
43	106		ABP552	Ábrányi-Balogh Péter				80,00			Pd/C	Reaction: 20 mL EtOH-ban gömblombikban felveszem a nitrovegyületet, hozzáadom a Pd/C-t, 40°C-on 30 per...
44	107		ABP5472	Varga Imre Károly	2018.03.14. 14:1...							Reaction: 20 mL THF és 10 mL deszt víz elegyében felvesszük az észtert, majd hozzáadjuk a szilárd NaOH-t. R...
45	108		ABP553	Varga Imre Károly								Reaction: 50 mL DMF-ben felvesszük a savat, majd kevertetés közben hozzáadjuk a szulfidot, és 80°C-ra melegítjü...
46	109		ABP554	Ábrányi-Balogh Péter	2018.03.22. 15:5...			25,00		2,00		Reaction: NaH is suspended in 10 mL of DMF, and phenol is added dropwise in 10 mL DMF. After 30 min, MeI is added. Stirred fo...

ELN_Reactions: 46 out of 46 rows.

And the answer is…

- Still in the test phase with all of the lab members
- Satisfying the claims of the research group

Special thanks

- For the **development**: Ákos Tarcsay, senior application scientist
- For the first **testing**: Ádám Kelemen, PhD student
- **To be here**: ChemAxon

Thank You for Your attention!