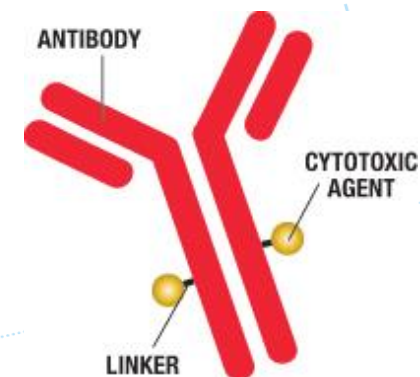


# IDBS & ChemAxon

Ian Peirson  
April 2018

# The Changing Landscape of Chemistry



... which leads to the strategic partnership between ChemAxon & IDBS

- Navigator
- Inbox
  - Root
    - 1. Chemistry
      - Example Expt (SAR)
      - Landing page
      - Project 1
        - EXP-Ian1183
          - (v. 2) Stoichiometry: Stoichiometry
          - EXP-Ian1185
            - (v. 2) Stoichiometry: Stoichiometry
            - (v. 1) Unknown: JMedChem.pdf
            - (v. 1) Unknown: 1H NMR.pdf
            - (v. 1) Unknown: Example Excel Spreadshe
            - (v. 1) Stoichiometry: Stoichiometry
          - EXP-Ian1209
          - EXP-Ian1210
          - EXP-Ian1211
          - EXP-Ian1212
          - EXP-Ian1391
          - EXP-Ian1392
          - EXP-Ian1394
          - EXP-Ian1412
          - EXP-Ian1413

EXP-Ian1185

Root / 1. Chemistry / Project 1 / EXP-Ian1185

Save As Review & Sign R

Title : EXP-Ian1185 Version Type : DRAFT

(v2) Stoichiometry: Stoichiometry

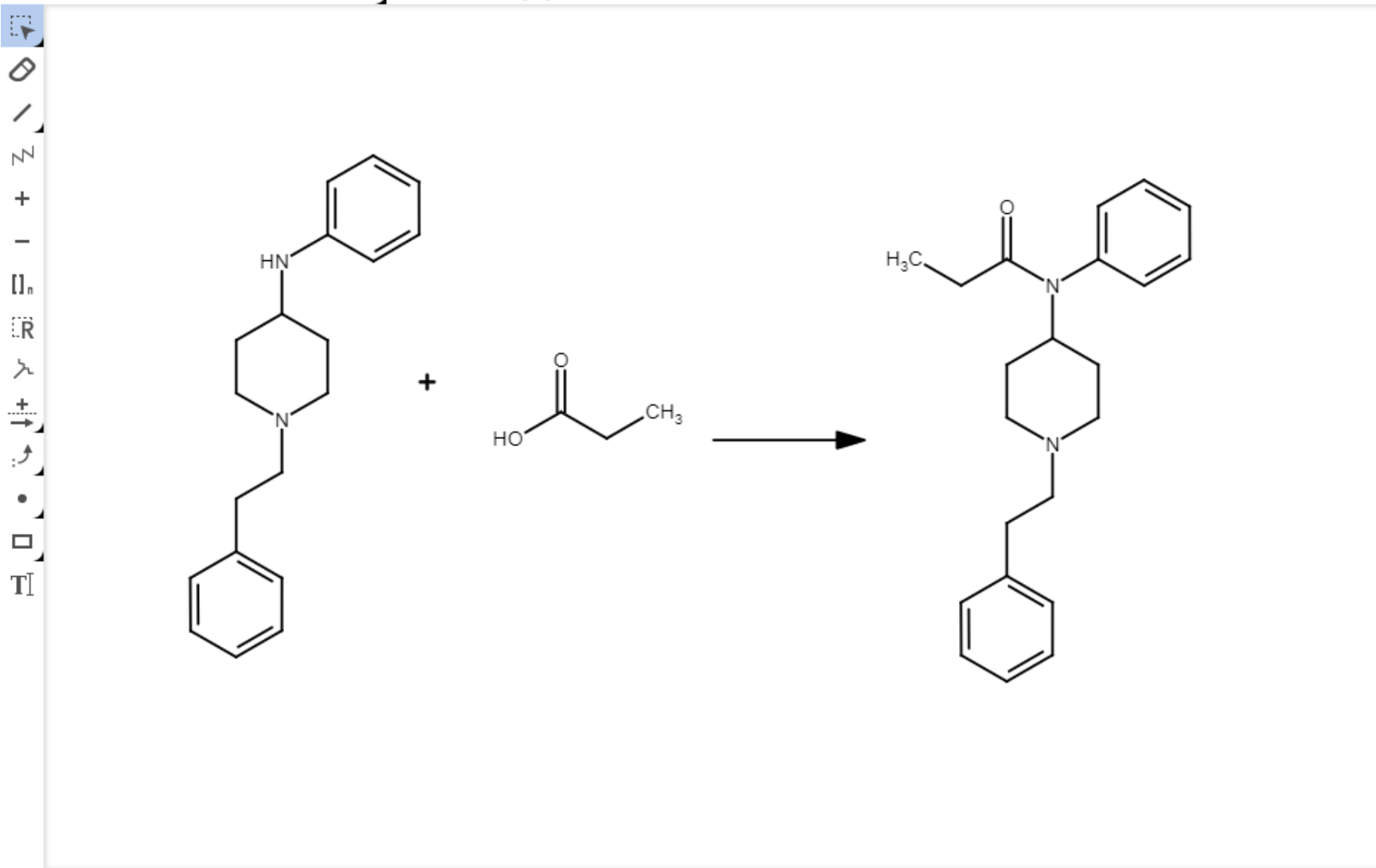
**Synthesis Table**

Total reaction mass: 29.037 g Total reaction volume: 99.958 mL

Reactants	Equiv.	Mass	Volume	Purity	Quantifier	n	Limit
(R1) 4-amino-2-methyl-5-(sec-butyl)pyrazole-3-carboxamide	1	10 g		100 %		50.954 mmol	✓
(R2) 2-isopropoxybenzoyl chloride	1.1	11.134 g	9.279 mL	100 %	1.2 g/mL	56.05 mmol	

Formula:  $C_9H_{16}N_4O$  MW: 196.254 g/mol

MarvinJS  
JCHEM



## Compliance checker



We have identified that some of the compounds have legal documents associated to them.

Last run on: 11 Apr 2018 18:26:19

Run compliance checker again

## fentanyl :

- IT Decreto del Presidente della Repubblica del 9 ottobre 1990, n. 309 TABELLA II SEZIONE A
- FR Arrête du 22 fevrier 1990 fixant la listedes substances classees comme stupefiants ANNEXE I
- DE Gesetz uber den Verkehr mit Betaubungsmitteln (Betaubungsmittelgesetz - BtMG) Anlage III
- AT Suchtgiftverordnung Anhang I
- US ARCOS NDC Dictionary File
- UK Misuse of Drugs Act Part I Class A
- IE MISUSE OF DRUGS REGULATIONS Class A
- US Controlled Substances Schedule I
- DK Bekendtgørelse om euforiserende stoffer Liste B

Compliance  
Checker



### Browser

CXN53

Expand All | Collapse All

CXN53

- CXN53A

CXN53-001

CXN53-003

CXN53-002

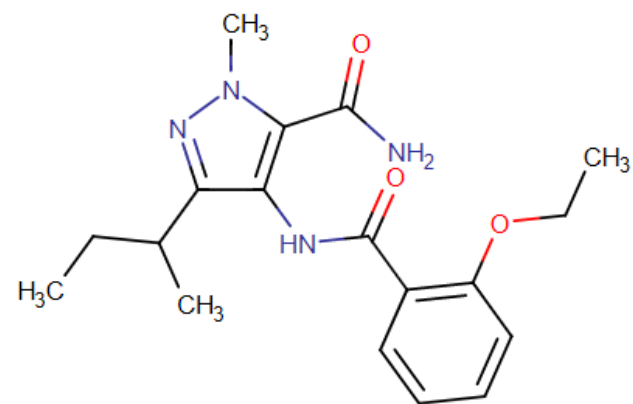
PCN: CXN53

Amend

More actions

Check

Single Structure



DATA

Chemically Significant Text

Enter any text value

### CXN53

Molecular Formula	C18H24N4O3
Mol Weight	344.415
User Specified Mol Weight	0
Created by	admin
Submitter	Ian
Created on	Sep 12th, 2016 18:17:22 UTC
Modified on	
Restriction	0

### Structure Checker



Analysis will trigger automatically when you start editing the structure.

Perform Quality Checks

Data Fields

Stereo Analyzer

### Additional Data

Default

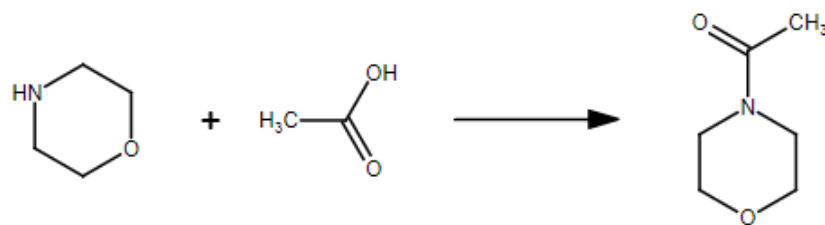
Stereochemistry

Geometric isomerism

Data fields that are not defined for this structure are automatically hidden. [Show all fields](#)

Remove fields

Chemistry  
Registration



Displaying the first enumerated reaction

REACTANT 1 (3)

REACTANT 2 (4)

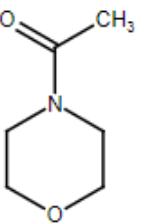
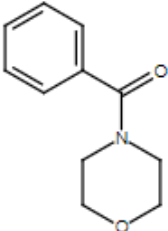
OTHER COMPONENTS (3)

PRODUCTS (12)

PROCEDURE

No products selected

Register

<input type="checkbox"/> Product	Structure	Run Number	LC Analysis	LC (sent)	LC (returned)	Registration	Comment
<input type="checkbox"/> EXP-Ian1209 - P-001	 Formula: C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub> MW (g/mol): 129.159	1	LCMS (tR): 1.48 min	Quantity: 0.48 g	Quantity: 0.25 g	Registered as: CXN103	Date: 9 Jan 2018
<input type="checkbox"/> EXP-Ian1209 - P-002	 Formula: C <sub>11</sub> H <sub>13</sub> NO <sub>2</sub> MW (g/mol): 191.23	1	LCMS (tR): 2.2 min	Quantity: 0.55 g	Quantity: 0.29 g	Registered as: CXN104	Date: 9 Jan 2018

Plexus Design  
(as input)

## Navigator



My Work

Favorites

Inbox

Root

1. Chemistry

Example Expt (SAR)

Landing page

Project 1

EXP-Ian1183

EXP-Ian1185

EXP-Ian1209

EXP-Ian1210

(v. 2) Biomolecule: Biomolecule

(v. 1) Biomolecule: Biomolecule

(v. 1) Biomolecule: Biomolecule

EXP-Ian1211

EXP-Ian1212

EXP-Ian1391

EXP-Ian1392

EXP-Ian1394

EXP-Ian1412

EXP-Ian1413

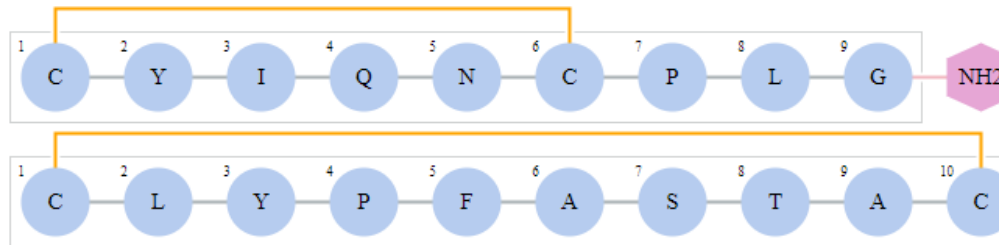
EXP-Nathalie1283

## EXP-Ian1210

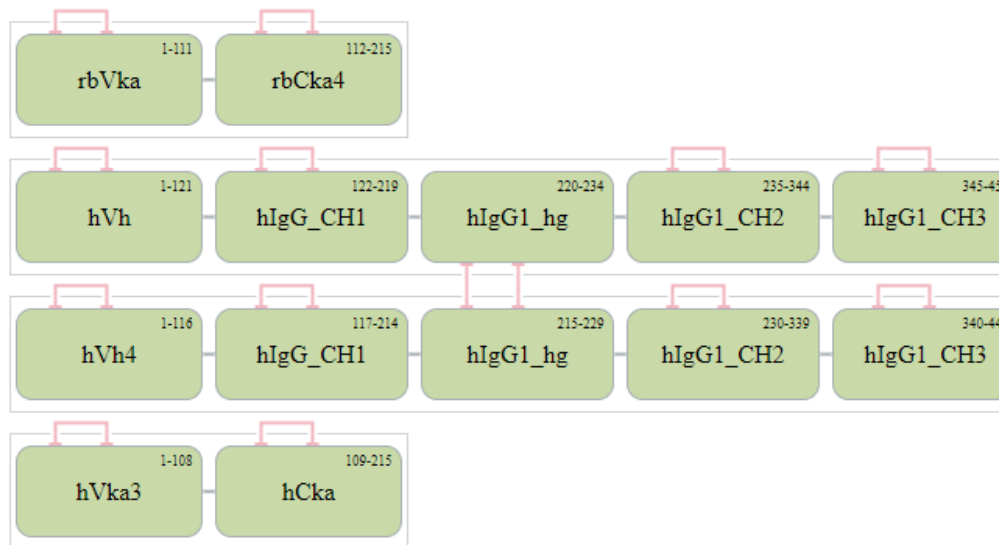
Root / 1. Chemistry / Project 1 / EXP-Ian1210



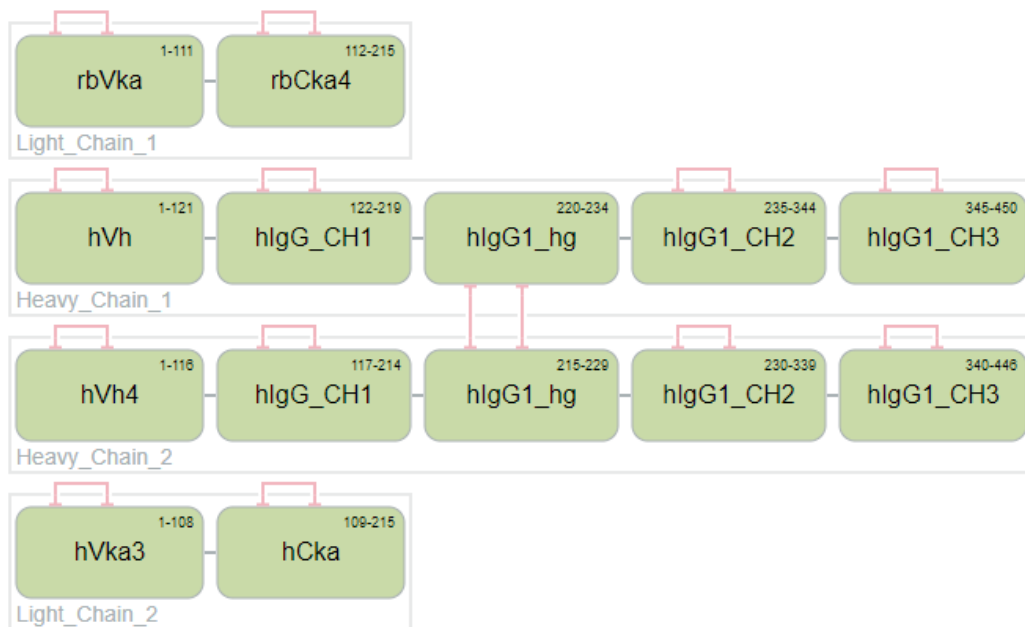
(v2) Biomolecule: Biomolecule



(v1) Biomolecule: Biomolecule



BioEddie



Details - Macromolecule

MOL export module is not available.

Library

Search

Peptide CHEM Nucleic acid BLOB

X	A	C	D
E	F	G	H
I	K	L	M
N	O	P	Q
R	S	T	V
W	Y	U	dA
dC	dD	dE	dF
dH	dI	dK	dL
dM	dN	dP	dQ
dR	dS	dT	dV
dW	dY	Aib	B-Ala

Tools

Registration

Register the biomolecule to the biology registration system

Register

BioMolecule Toolkit



# Where are we going with joint development?

- Standardiser
- Plexus Design
- BioMolecule Toolkit
- ChemCurator

## How are we going to get there?

**Voice of the customer!** We hold regular chemistry forums in Boston & Munich to discuss ideas for product development

