

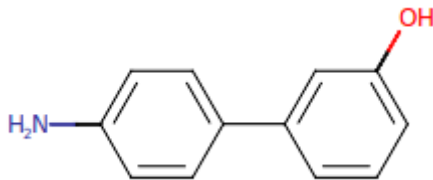
# NAMING

Daniel Bonniot de Ruisselet

UGM / San Diego / 2015

# ChemAxon's Naming Suite

Constantly improving and innovating  
Major recent features and improvements:



4'-amino-[1,1'-biphenyl]-3-ol

- Improved English, Chinese and Japanese Name and Document to Structure
- Plexus Mining and Document annotation

# Document annotation

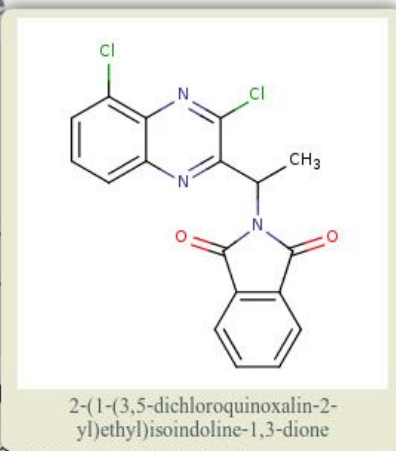
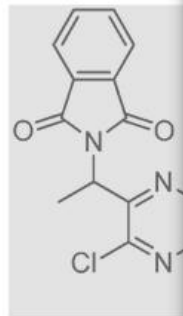
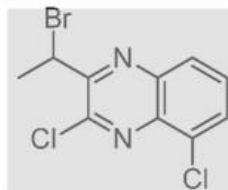
WO 2013/152150

PCT/US2013/035203



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2-(1-(3,5-dichloroquinoxalin-2-yl)ethyl)isoindoline-1,3-dione



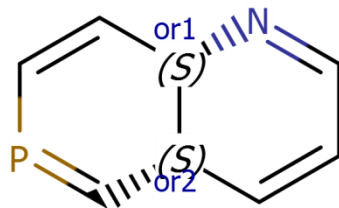
To a solution of 2-(1-bromoethyl)-3,5-dichloroquinoxaline (1.00 mol) in DMF (8.2 L) was added potassium phthalimide (1.21 Kg, 6.54 mol). The reaction

5 mixture was stirred for 3 h. At this time LC-MS analysis showed that the reaction

# Document annotation

- PDF, Text, Patent XML, HTML → Chemically annotated HTML
- Use cases:
  - Part of your custom application or website
  - ChemCurator
  - Your documents inside Plexus Mining
  - <http://d2db.chemaxon.com>

# IUPAC nomenclature conundrum

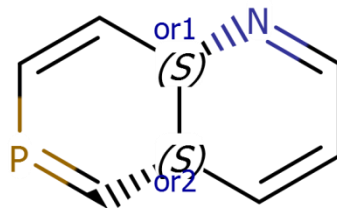


Why generate a name?

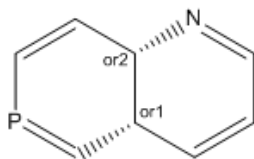
- Publish an article
- Apply for a patent
- Internal purposes (identify each compound)

2014: “Nobody solved it yet on the market, but ChemAxon is the closest among all the solutions.”

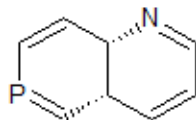
# IUPAC nomenclature conundrum



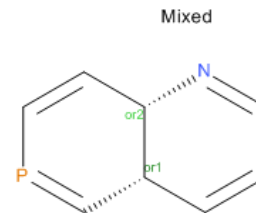
2014: “Nobody solved it yet on the market, but ChemAxon is the closest among all the solutions.”



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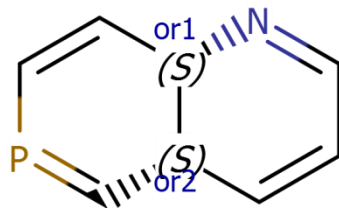


(4a*S*,8a*S*)-4a,8a-dihydrophosphinino[4,3-*b*]pyridine

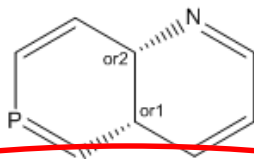


rel-(4a*S*,8a*S*)-4a,8a-dihydrophosphinino[4,3-*b*]pyridine

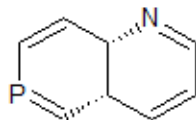
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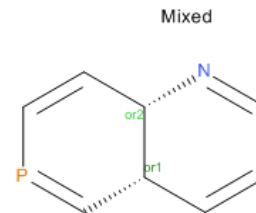
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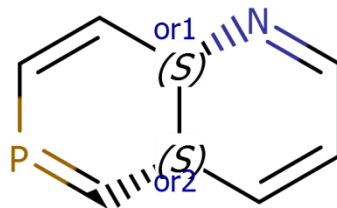


(4a*S*,8a*S*)-4a,8a-dihydrophosphinino[4,3-*b*]pyridine

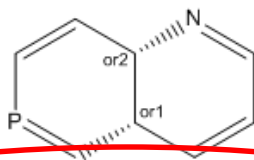


rel-(4a*S*,8a*S*)-4a,8a-dihydrophosphinino[4,3-*b*]pyridine

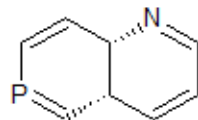
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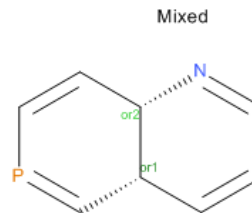
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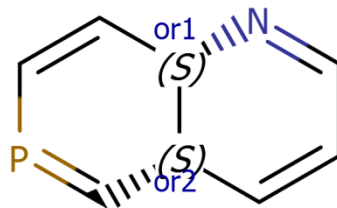
(4a*S*,8a*S*)-4a,8a-dihydrophosphinino[4,3-*b*]pyridine



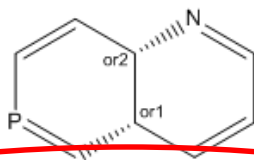
rel-(4a*S*,8a*S*)-4a,8a-dihydrophosphinino[4,3-*b*]pyridine



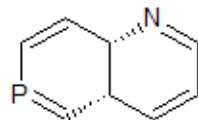
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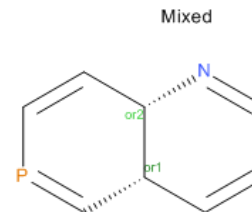
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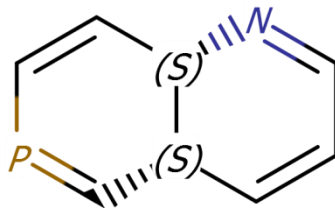


(4a*S*,8a*S*)-4a,8a-dihydrophosphinino[4,3-*b*]pyridine



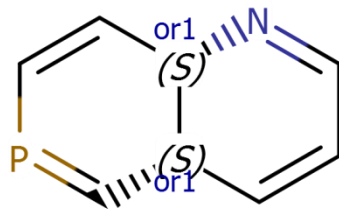
rel-(4a*S*,8a*S*)-4a,8a-dihydrophosphinino[4,3-*b*]pyridine

# IUPAC nomenclature conundrum



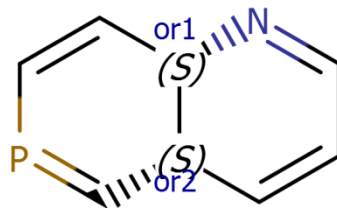
(4a*S*,8a*S*)-4a*H*,8a*H*-phosphinino[4,3-*b*]pyridine

# IUPAC nomenclature conundrum



rel-(4aR,8aR)-4aH,8aH-phosphinino[4,3-b]pyridine  
(4aR\*,8aR\*)-4aH,8aH-phosphinino[4,3-b]pyridine

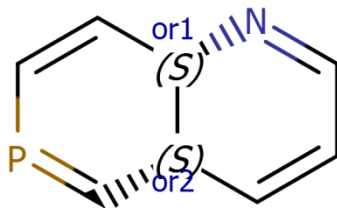
# IUPAC nomenclature conundrum



?

Structure representable using MOL V3000 format  
IUPAC standard silent about the name

# IUPAC nomenclature conundrum



(4aR\*,8aR\*\*) -4aH,8aH-phosphinino[4,3-b]pyridine

ChemAxon extension

Natural extension of the existing convention

Solves our customer's problem

Hopefully standardized in the future

# ChemAxon's Naming Suite

Constantly improving and innovating  
Reactive to customer's needs

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THANK YOU