ChemAxon

NAMING

Daniel Bonniot

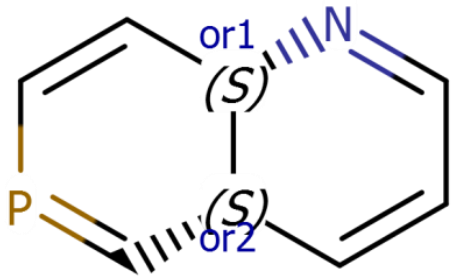
UGM Budapest 2015

NAMING

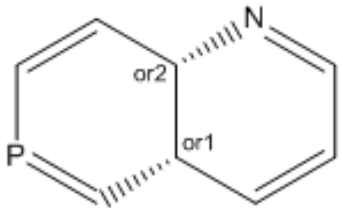
Name ↔ Structure

Document annotation

IUPAC nomenclature conundrum



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



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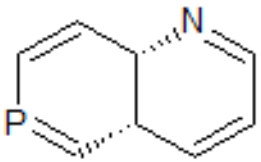
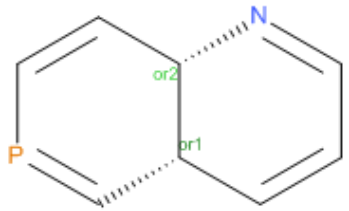


(4a*S*,8a*S*)-4a,8a-dihydrophosphinino[4,3-*b*]pyridine

Mixed



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

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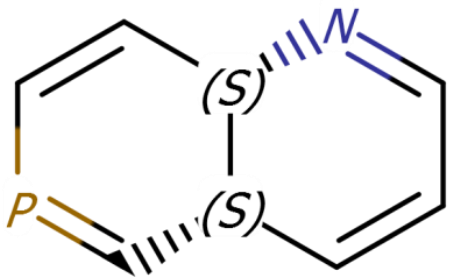
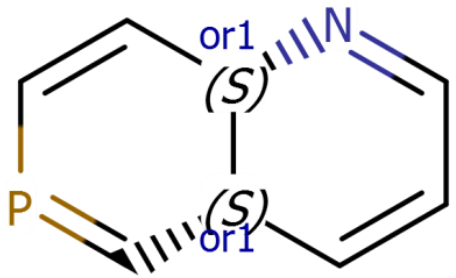
IUPAC nomenclature conundrum



(4aS,8aS)-4aH,8aH-phosphinino[4,3-b]pyridine

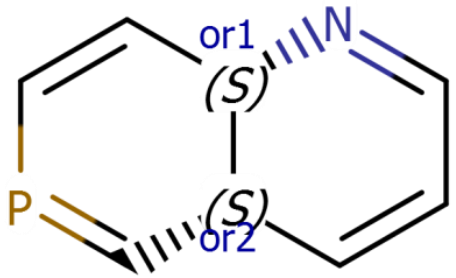
IUPAC nomenclature conundrum



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

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

IUPAC nomenclature conundrum



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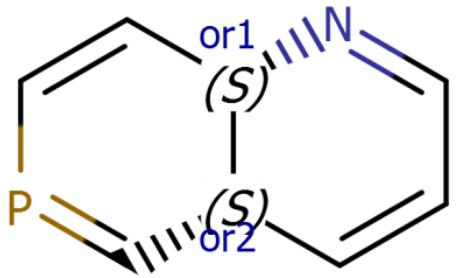
Structure representable using MOL V3000 format

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

Hopefully standardized in the future

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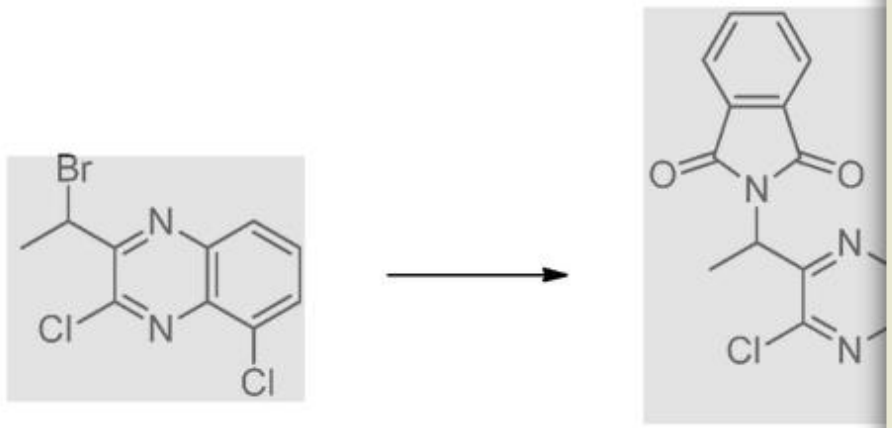
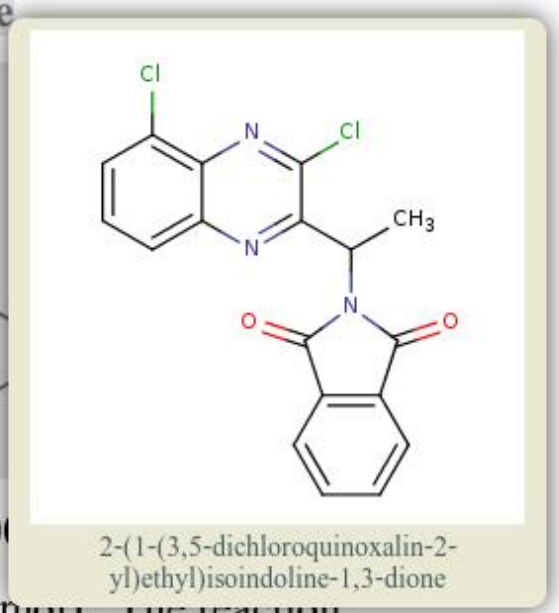
Document annotation

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





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

To a solution of 2-(1-bromoethyl)-3,5-dichloroquinoxaline (1.0
DMF (8.2 L) was added potassium phthalimide (1.21 Kg, 6.54 mol). The reaction
mixture was stirred for 3 h. At this time LC-MS analysis showed that the reaction

Document annotation

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