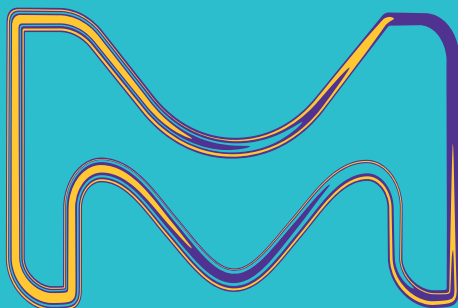


Millipore Sigma – InChi

Bret Daniel – August 2017

Discovery Chemicals & Informatics Lead

MilliporeSigma is a business of Merck KGaA, Darmstadt, Germany



**Millipore
SIGMA**

Background

- Sigma Aldrich acquired by Merck KGaA – Nov. 2015 (MilliporeSigma in NA)
- Sigma Aldrich became InChi Associate member - Nov. 2015
- www.sigmaaldrich.com releases display of InChi(Key) – Jan 2017
- Discovery Chemistry & Services
 - SLN shop
 - 342M+ unique structures (iResearch Library)
 - 142M+ have InChi Code/Key assignments (ongoing)
 - Aldrich Market Select began support for InChi – Jun 2013 (www.aldrichmarketselect.com)
- Currently utilize the standard InChi (InChi=1S/)

SIGMA-ALDRICH is now **MILLIPORE SIGMA**

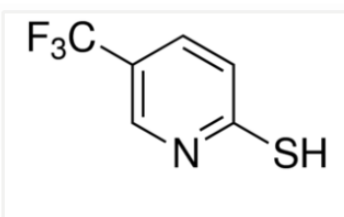
590762 ALDRICH
5-(Trifluoromethyl)pyridine-2-thiol
97%
Synonym: 5-(Trifluoromethyl)-2-mercaptopyridine, 5-(Trifluoromethyl)-2-pyridinethiol

SDS

CAS Number 76041-72-0 | Empirical Formula (Hill Notation) C₆H₄F₃NS | Molecular Weight 179.16
MDL number MFCD00128893 | PubChem Substance ID 24881297

Properties

Related Categories	Building Blocks, C6, Chemical Synthesis, Heterocyclic Building Blocks, Pyridines More...
InChi Key	YFSCXL SUZZXNHU-UHFFFAOYSA-N
assay	97%
mp	154-159 °C(lit.)
storage temp.	2-8°C



The image shows a screenshot of the Sigma-Aldrich product page for 5-(Trifluoromethyl)pyridine-2-thiol. It includes the product name, synonyms, CAS number, empirical formula, molecular weight, MDL number, and PubChem ID. A table lists properties such as related categories, InChi key, assay, melting point, and storage temperature. A chemical structure is also displayed, showing a pyridine ring with a trifluoromethyl group at the 5-position and a thiol group at the 2-position.

www.aldrichmarketselect.com/inchishow.asp?strid=406191775

InChi Code

InChi Code for Structure Id 406191775

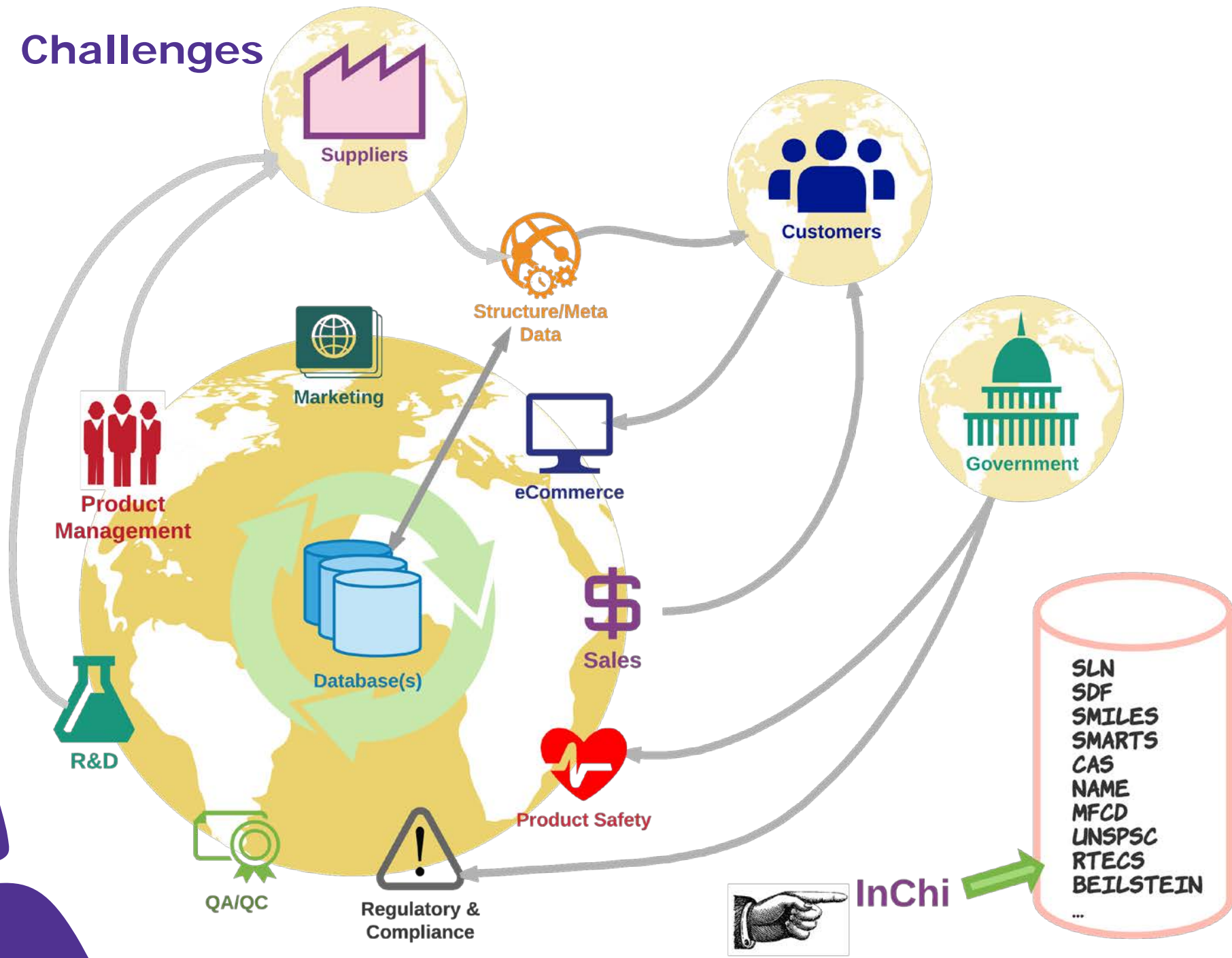
InChi=1S/C24H22CIN3O2/c25-21-12-18(8-5-17(21)13-26)28-23(14-3-1-2-4-14)20-10-6-15-11-16(24(29)30)7-9-19(15)22(20)27-28/h5,7-9,11-12,14,23,27H,1-4,6,10H2,(H,29,30)/t23-m/s1

SIGMA-ALDRICH

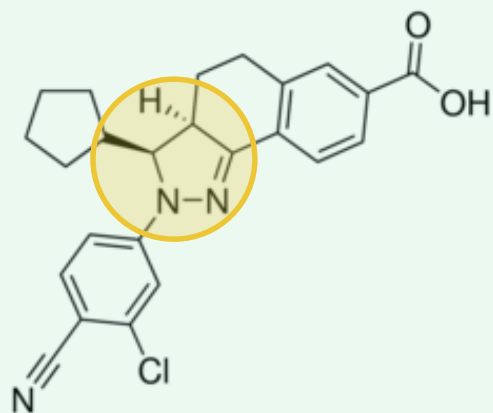
The image shows a screenshot of the Aldrich Market Select website displaying the InChi code for a specific structure. The URL is www.aldrichmarketselect.com/inchishow.asp?strid=406191775. The page features a blue header with the text 'InChi Code' and a red footer with the 'SIGMA-ALDRICH' logo. The main content area displays the InChi code for structure ID 406191775, which is InChi=1S/C24H22CIN3O2/c25-21-12-18(8-5-17(21)13-26)28-23(14-3-1-2-4-14)20-10-6-15-11-16(24(29)30)7-9-19(15)22(20)27-28/h5,7-9,11-12,14,23,27H,1-4,6,10H2,(H,29,30)/t23-m/s1.



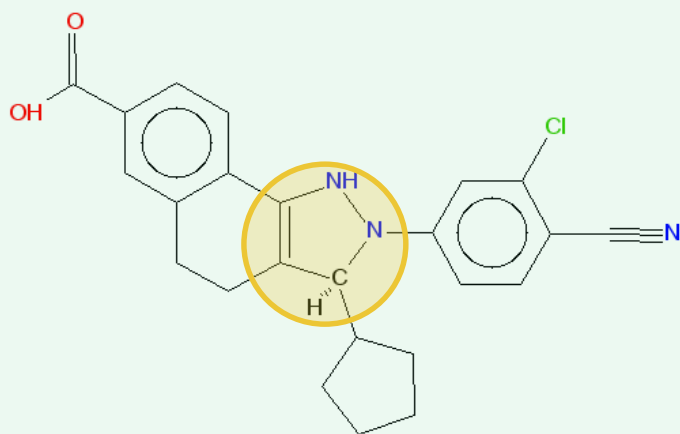
Challenges



Next Steps



XNULRSOGWPPFBL-REWPJTCUSA-N



ONEWULDKRWPYMP-QHCPKHFHSA-N

- **Embrace**
Integrate the InChi into existing data programs across organization
- **Educate**
Bring awareness to internal and external groups/suppliers/customers, etc.
- **Communicate**
Address questions and concerns

Moving forward

- Adoption confidence – Round trip structures with existing tools
- Adopt workflows to establish early structure creation and identification (*Safety, Regulatory, etc.*)
- Normalization evaluation (100+ steps)
- Mixtures
- Polymers

Beyond Chemistry

- DELs?
- Helm Notation



Q&A