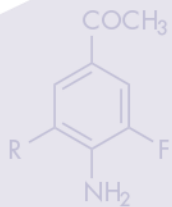
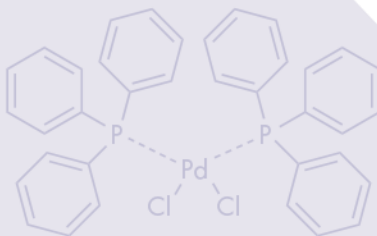


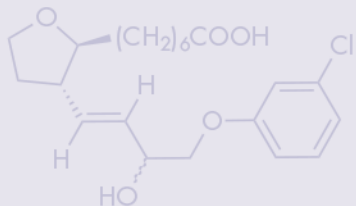
Dedication



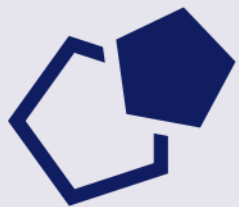
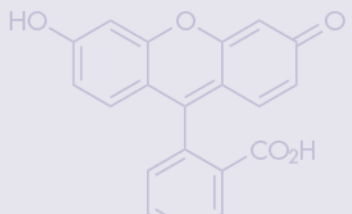
Integrity



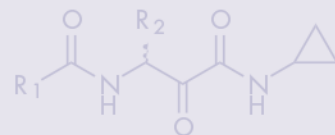
Development



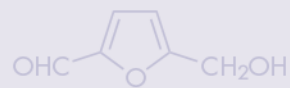
Performance



# NCK

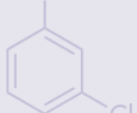
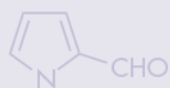
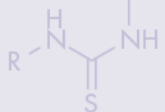


Passion



Minimized risk

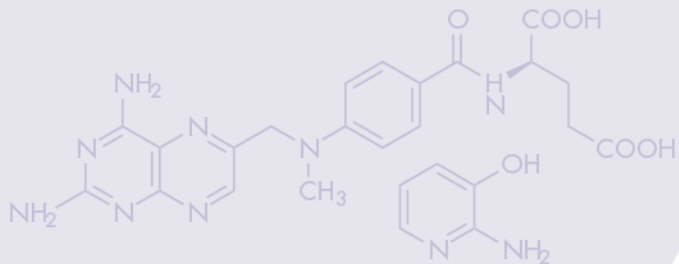
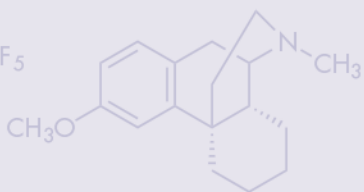
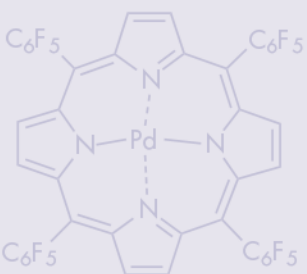
Focus



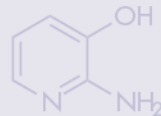
## BRIDGING THEORY AND KNOW-HOW

Life science

- science at work



Progression



# Migrating a legacy platform from the “DOS age” to Instant JChem

## - Is ChemLocator next level?

- ◆ *Brian Kreiser, Ph.D.*
- ◆ *Project Manager*
- ◆ *NCK A/S (Denmark)*

## THE STORY SO FAR...

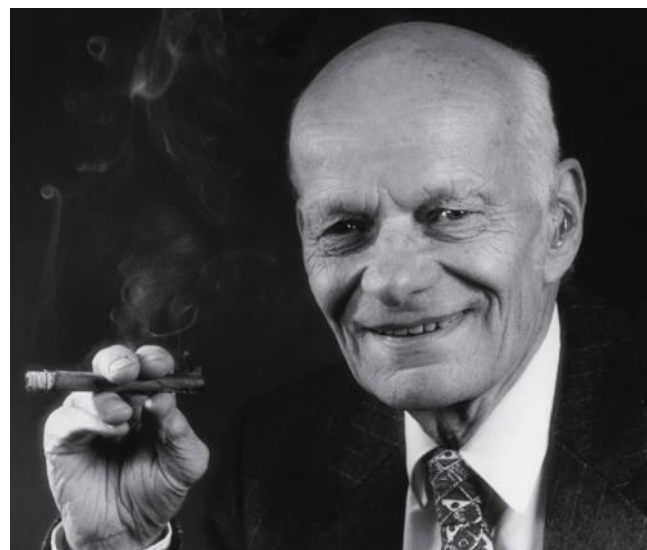
The founder of our company, NCK, Dr Niels Clauson-Kaas, started his career at the universities in Copenhagen, Zürich and Haifa. In 1949 he was offered a position as head of an industrial organic synthesis laboratory in Denmark.

In 1956 he decided to start his own company, focusing on research and development in organic synthesis, providing contract services to the chemical industry.

## INDEPENDENT COMPANY

In 1983, a foundation was established to facilitate the buyout of Niels Clauson-Kaas.

The objective was evident: To build a sustainable company, and continue to have an inspiring work environment.



# OUR FOUNDATION

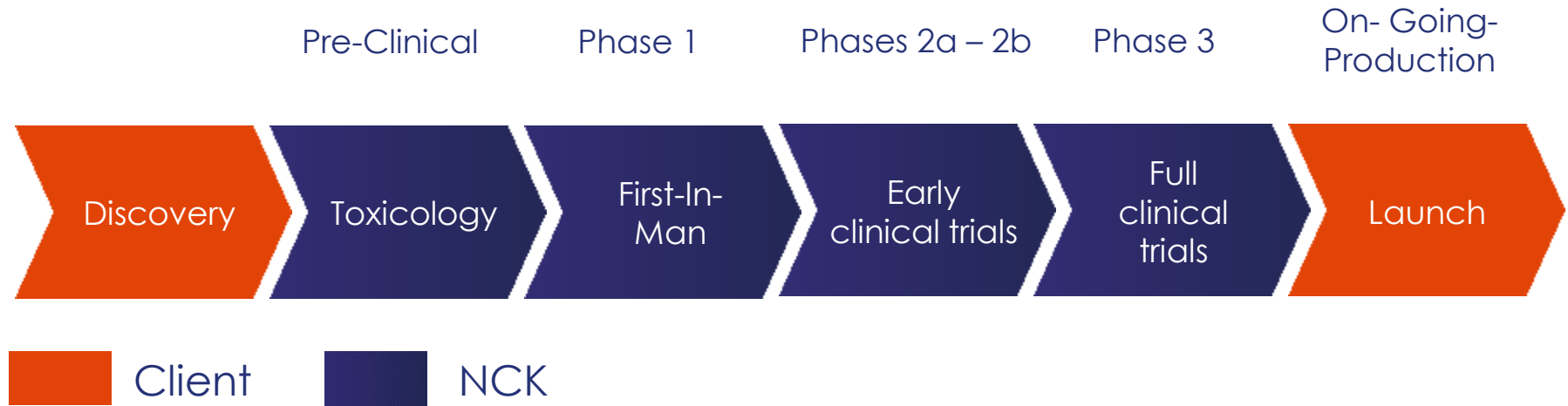
*- a technology based company*

- ◆ 62 Years' Experience  
in Synthetic Organic Chemistry
- ◆ Process Development / Up-Scaling
- ◆ Lab to Pilot Scale Syntheses
- ◆ API Manufacturing according to cGMP
- ◆ Analytical Development and Validation
- ◆ Stability Studies
- ◆ Genotoxic Impurities / Method Development
- ◆ Technology Transfer
- ◆ Approx. 50% of our projects over a 5 years period  
are for oncology therapeutics



# Imagine if...

- your new potential drug were to enter the development stage..

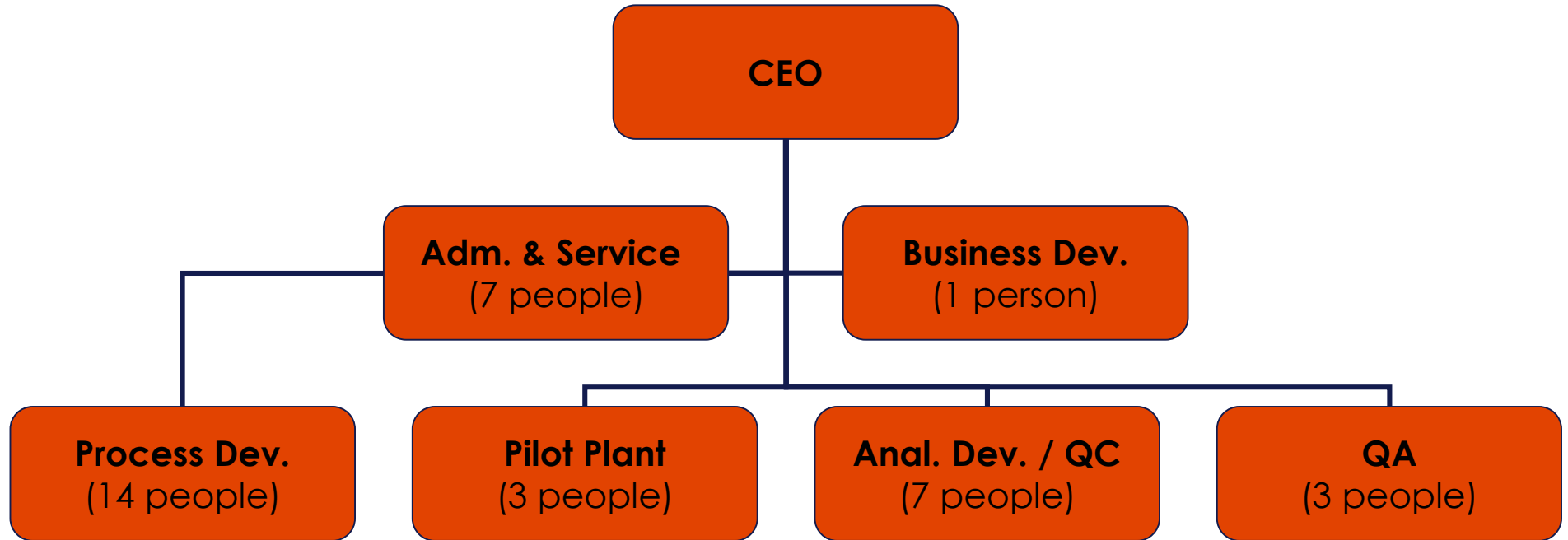


..you will need a trustful CMC partner who can support, guide and

- structure a project to meet the various milestones
- provide the right solution in high quality
- deliver with the world's best track record

# ORGANIZATION

March 2018



# DATABASE SETUP

- ◆ *Work on the reaction Database was initiated in 1990*
- ◆ *One of the best choices of database software in the "DOS age" was ChemBase*
- ◆ *> 8,000 Reactions were stored in the database, which was maintained until 2014.*




# CHEMBASE

DOSBox 0.74, Cpu speed: 3000 cycles, Frameskip 0, Program: CBASE

ChemBase Main Menu RXN FRM

Clear Retrieve Search Edit Update View Exit

ID	3671	Topic	05764	CK	01097	Date	25.03.91	
Reactant	C7 H7 N O2; C6 H12 O3			Product	C11 H9 N O2			
Reagent								
								
CAS-RN							(%)	:
Proj.				Rep.				
Keywords							Anal.	:
							Lit.	:

CK-RXN: 7881 Searching: 7881/7881 List A: 1/2 B: 1 F5=FxKeys





# NCK ISSUES WITH CHEMBASE

- *Only few people in the company are comfortable using DOS today*
- *Important chemical know-how not fully exploited as the project managers do not check our reaction database*
- *The DOS platform is obsolete*
- *The data could not be exported into a new windows based chemical database*



# DATABASE TRANSFORMATION

- *ChemAxon offered to test our ChemBase data, free of charge*
- *A pilot project was performed on a small part of the database – with success*
- *The full ChemBase database was converted to Instant Jchem.*



# INSTANT JCHEM

The screenshot displays the Instant JChem 6.2.2 software interface. The main window shows a chemical reaction scheme where a cyclic acetal reacts with 4-aminobenzoic acid to form a product where the amine group is cyclized into a pyrrole ring. The interface includes a menu bar (File, Edit, View, Search, Data, Lists, Chemistry, Tools, Window, Help), a toolbar, and a sidebar with project navigation options. A data table at the top right contains the following information:

TOPIC	PROJECT	CK PRODUCT	YIELD	ENTRY DATE	Last Update
5764		1097		25-03-1991	28-02-2014

Below the reaction scheme, there are input fields for KEYWORDS and REAGENT. On the right side, there are boxes for Calculated Reactant Formula (C6H12O3, C7H7NO2) and Calculated Product Formula (C11H9NO2), along with an Update Formulae and MW button. At the bottom, an Intermediate table shows 2 out of 7,681 rows and 0 out of 279 intermediates. An Output window titled 'Groovy' is also visible.



# ELECTRONIC DOCUMENTS

- ◆ *We have accumulated more than 3000 customer reports in various formats over the past 62 years.*
- ◆ *Several thousands of associated documents to various customer projects*



# ELECTRONIC DOCUMENTS

- *Can ChemLocator help us keeping track of our electronic data?*



# ELECTRONIC DOCUMENTS

The screenshot displays the ChemLocator web application interface. On the left, a 'Query' panel shows a chemical structure of 4-hydroxy-3-methoxybenzaldehyde. Below the structure are search controls: 'Structure search type' set to 'Substructure search', a 'Convert name to structure' section with an input field and 'Convert' button, and 'Free text conditions' with a dropdown menu and 'Add' button. A 'Search' button and 'Advanced Options' link are also present. At the bottom of the panel, it shows '55 documents on 5 pages', 'Query: 581 ms.', and 'Server time: 855 ms.'.

The main content area, titled 'ChemLocator v2.18.0126.2', displays search results. The first result is a 'DOCX' document named 'Forside\_Genzada', showing two chemical structures and the file path: \\nck\alle\rapporter\_LFORSIDE\Genzada\Forside\_Genzada.docx. The second result is another 'DOCX' document named 'Genzada\_summary\_4', showing two chemical structures and the file path: \\nck\alle\rapporter\Genzada\Genzada\_summary\_4.docx. The third result is a 'PDF' document named 'Genzada\_summary\_3', showing three chemical structures and the file path: \\nck\alle\rapporter\Genzada\Genzada\_summary\_3.pdf. The fourth result is a 'DOCX' document named 'Genzada\_summary\_3', showing two chemical structures.

# ELECTRONIC DOCUMENTS

*Further development on-going with ChemAxon*

- *Connect ChemLocator to the Instant JChem database.*
- *Create links to ChemLocator from molecular structures found via searches in Instant JChem.*
- *Make ChemLocator able to search for reactions.*



# CONCLUSION

- *Successful transfer of the ChemBase database.*
- *Project Managers are now actively searching and adding entries to the database for information.*
- *ChemLocator has greatly enhanced our ability to locate electronic documents.*
- *ChemLocator will greatly improve the value of our Instant JChem database, when electronic documents can be located via ChemLocator integration.*

